Correlated Reference States and Effective Hamiltonians in the IMSRG Framework

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& Department of Physics and Astronomy
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(Multi-Reference) In-Medium Similarity Renormalization Group

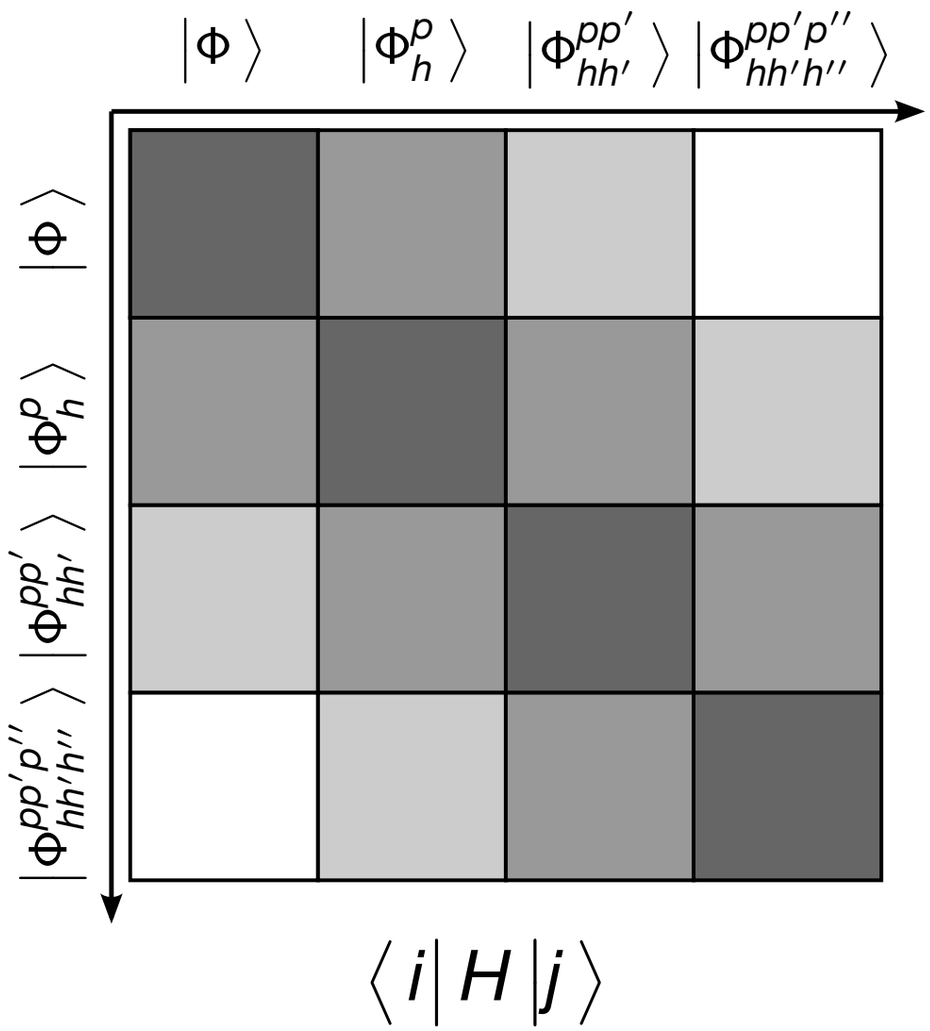
H. H., Phys. Scripta, Phys. Scripta 92, 023002 (2017)

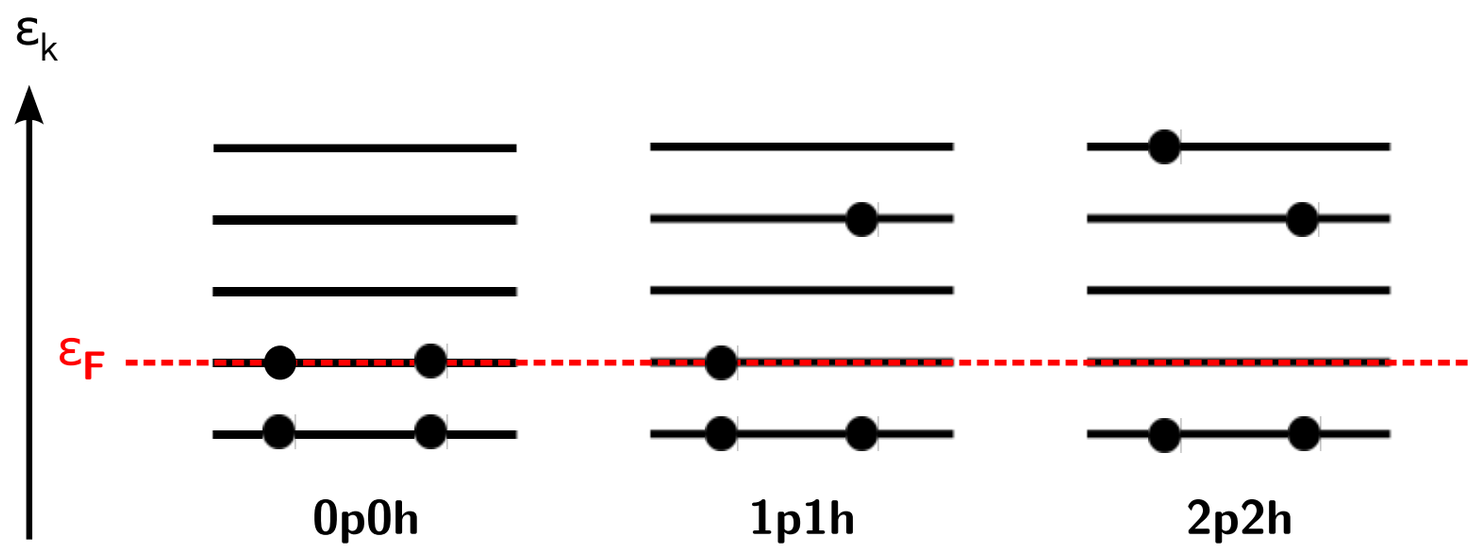
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

H. H., S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

Transforming the Hamiltonian

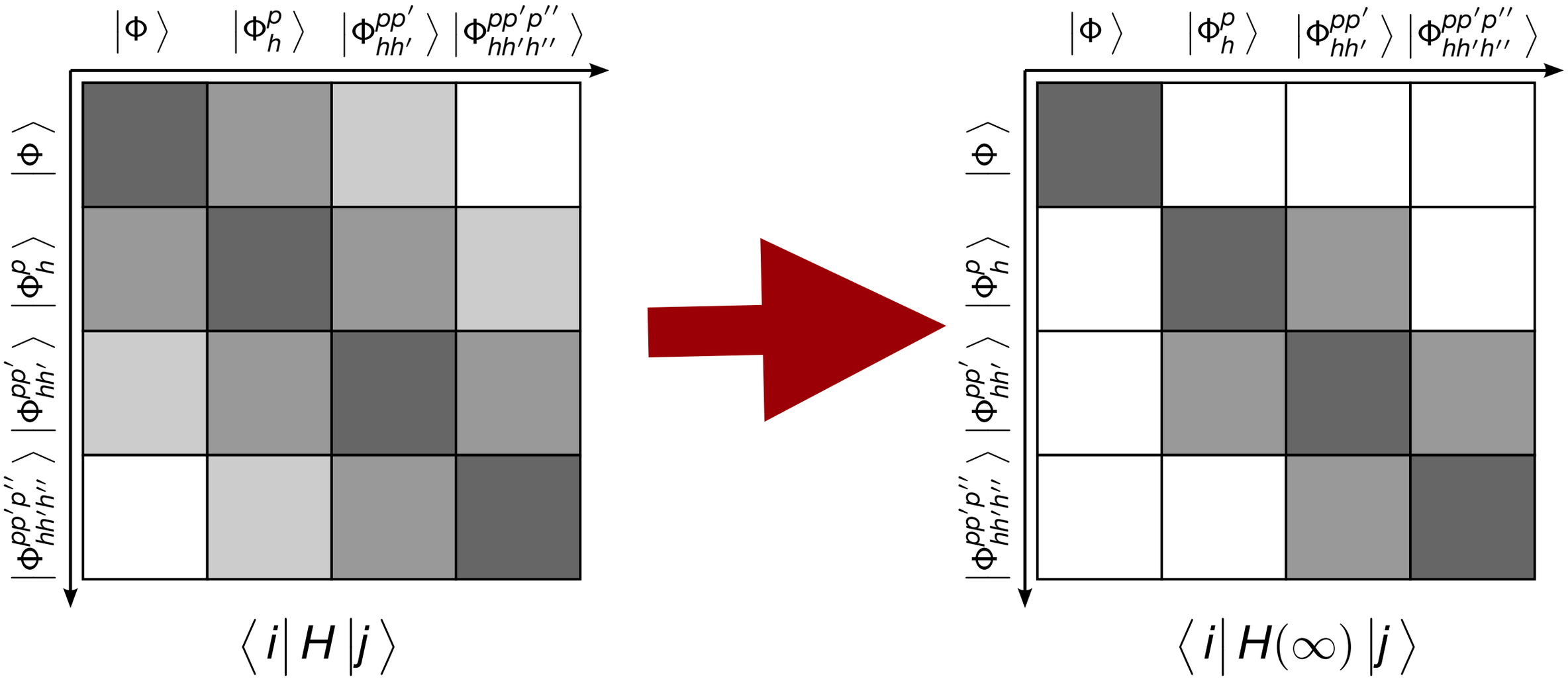




excitations relative to reference state: **normal-ordering**

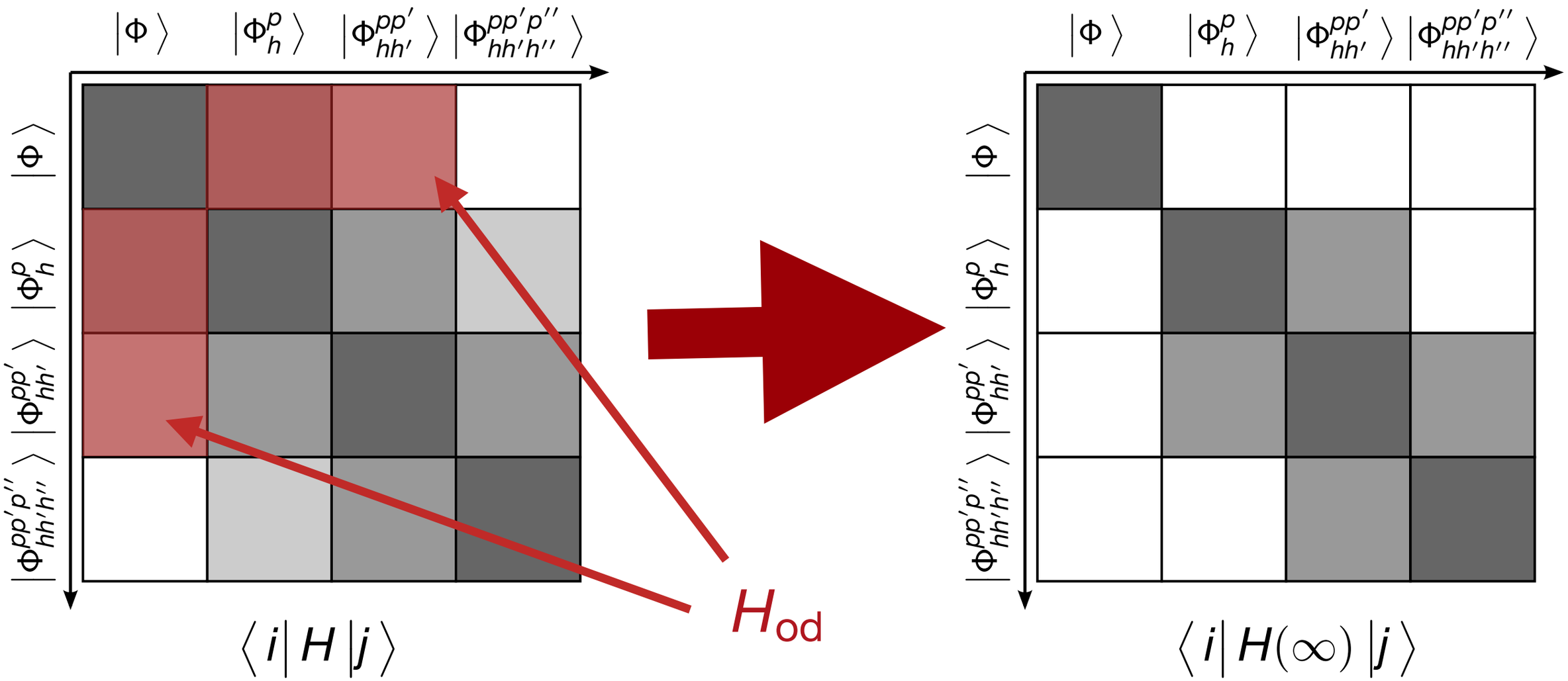
- reference state: **single Slater determinant**

Decoupling in A-Body Space



aim: decouple reference state $|\Phi\rangle$
from excitations

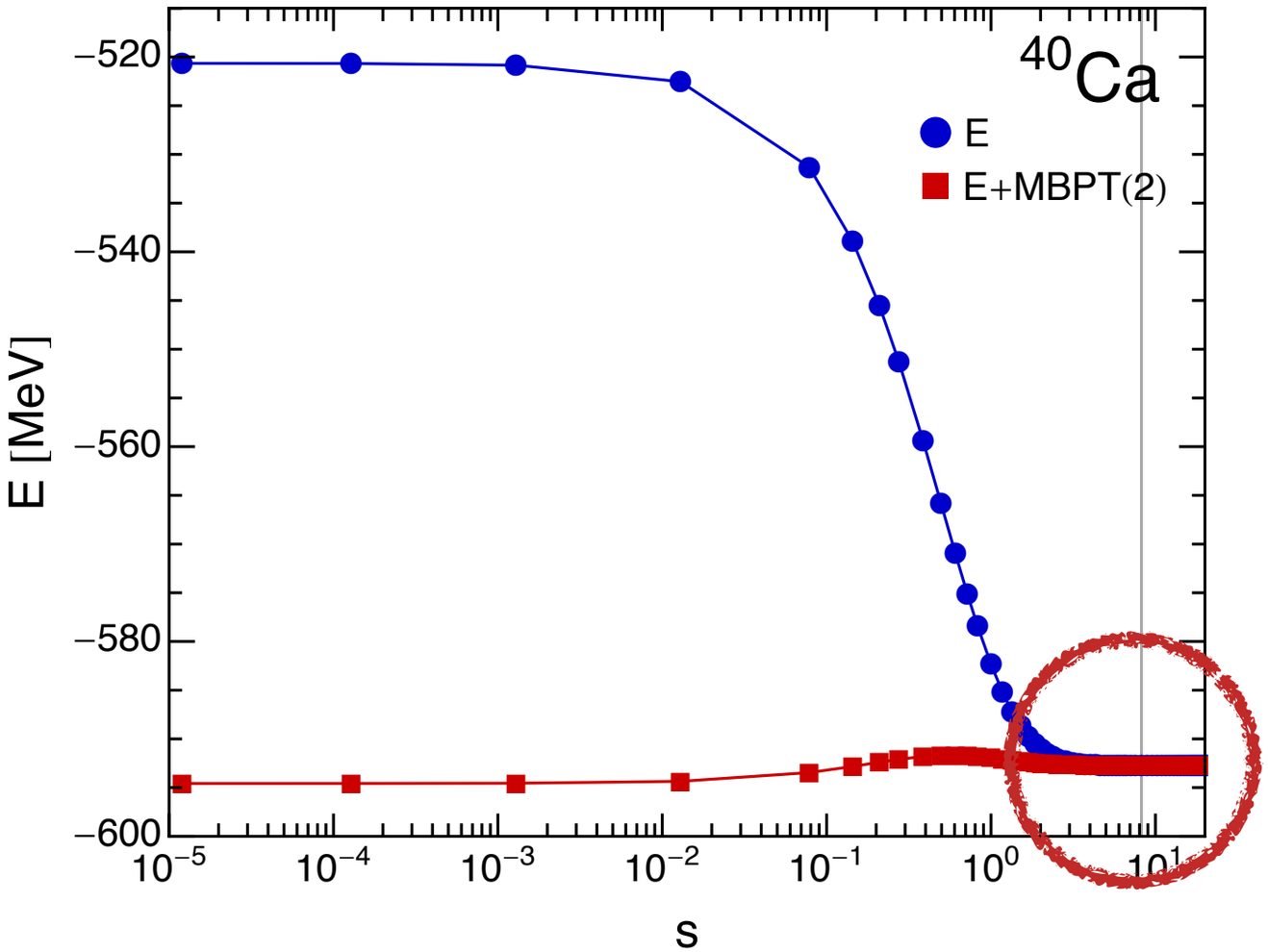
Flow Equation

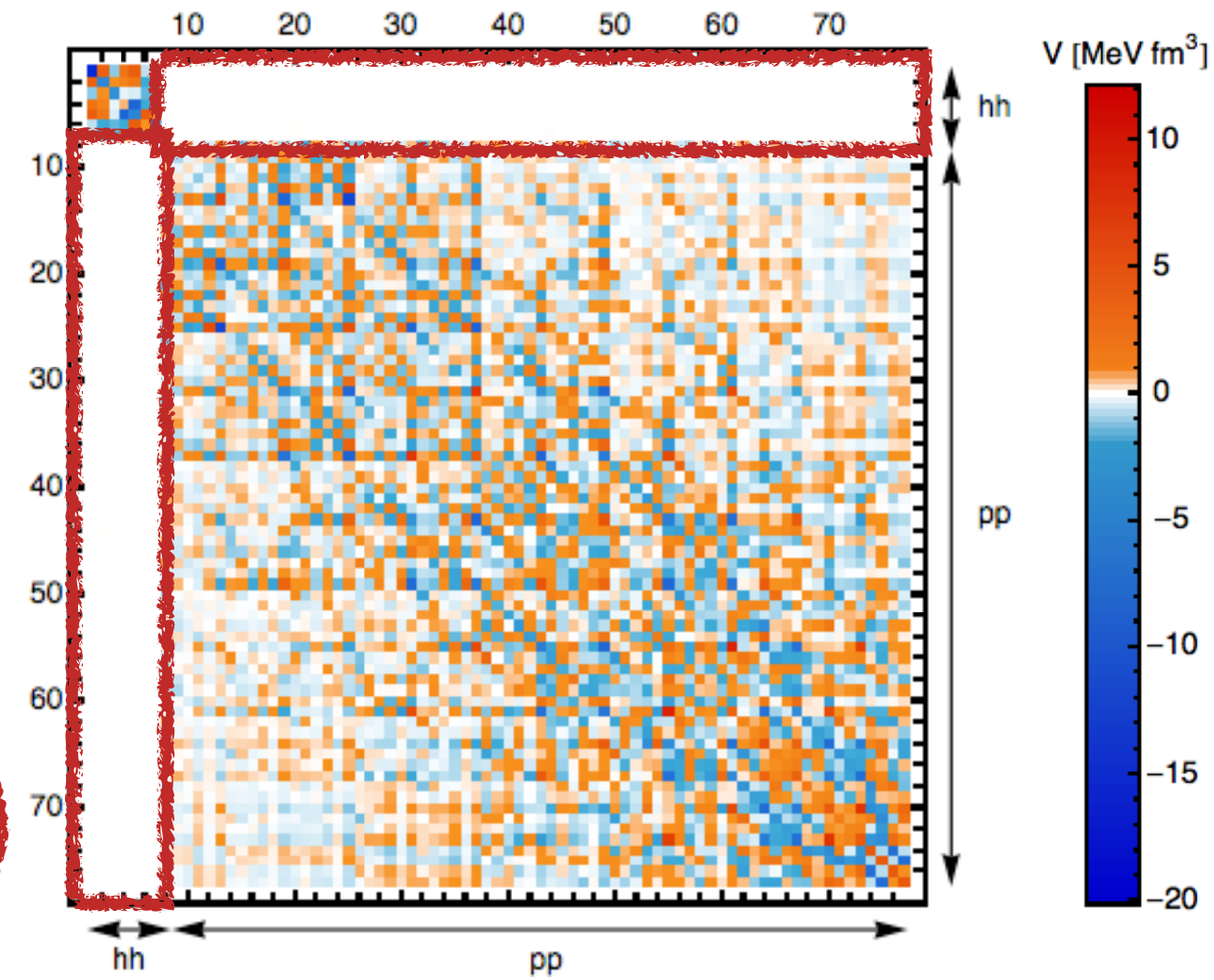


$$\frac{d}{ds}H(s) = [\eta(s), H(s)]$$

Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

Decoupling



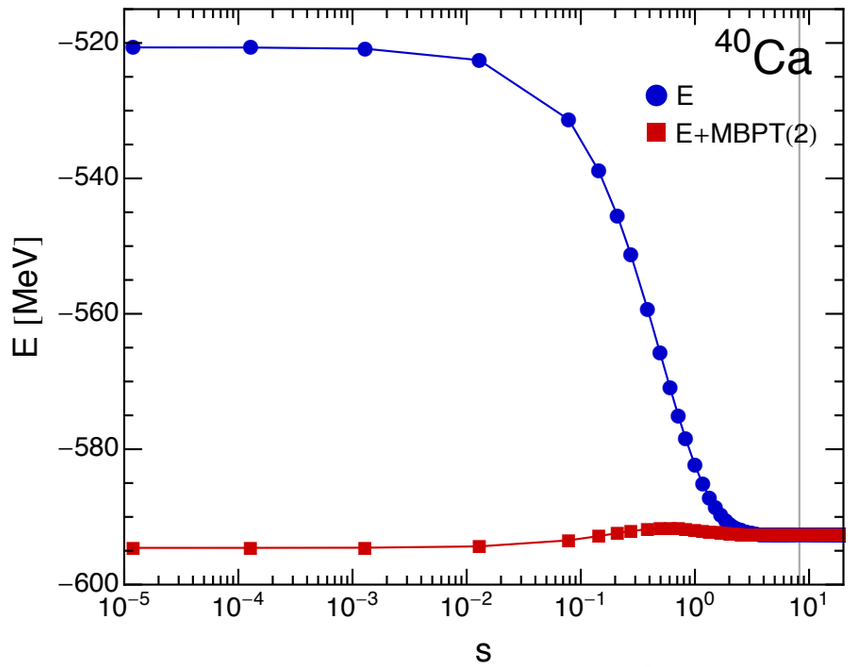


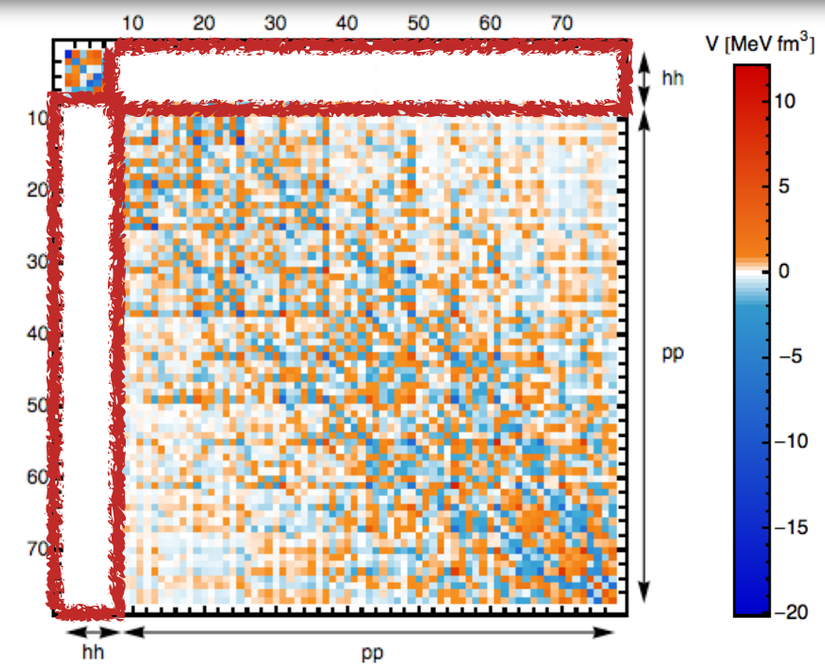
N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Decoupling





N3LO, $\lambda = 2.0$ fm^{-1}, $e_{\mathrm{Max}} = 8$

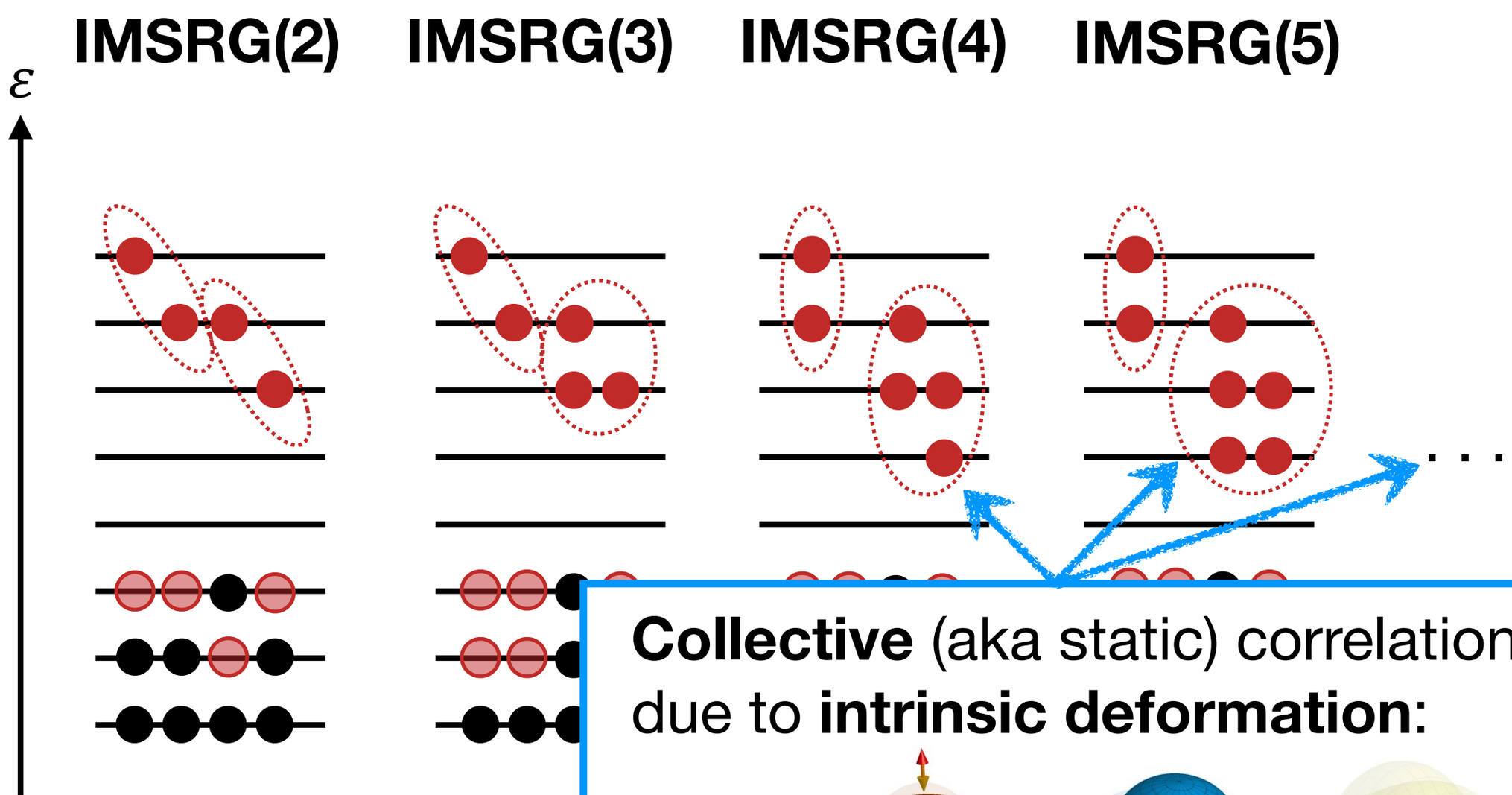
- absorb correlations into **RG-improved Hamiltonian**

$$U(s)HU^{\dagger}(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

- reference state is ansatz for transformed, **less correlated** eigenstate:

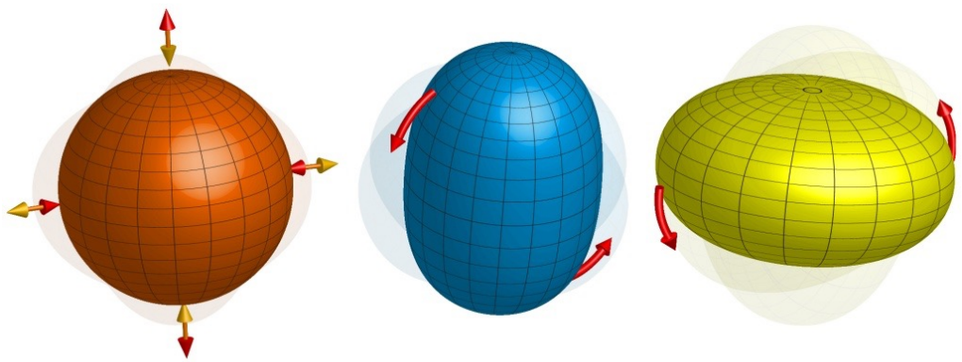
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

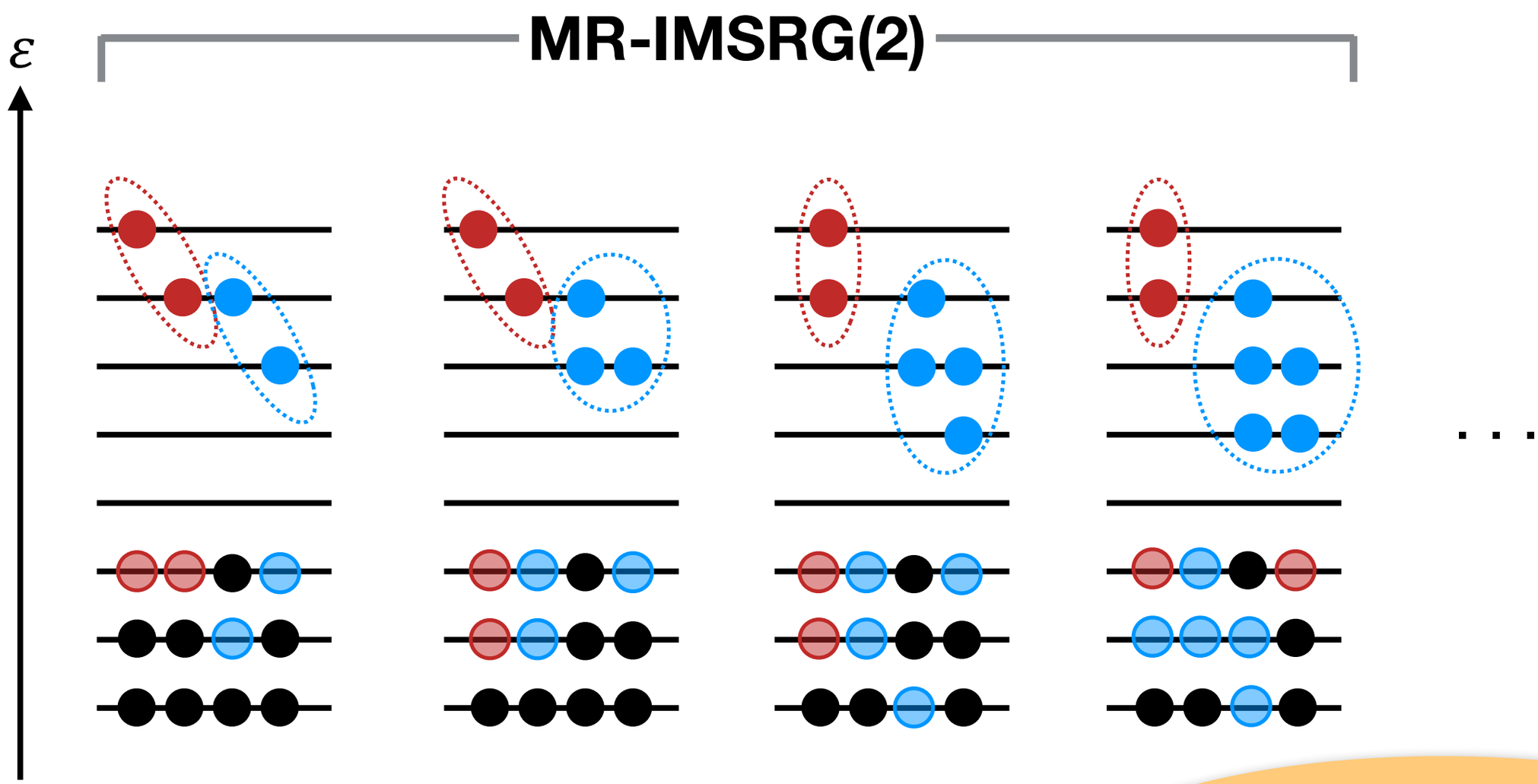


“standard” IMS
Slater determinan

Collective (aka static) correlations, e.g. due to **intrinsic deformation**:



Correlated Reference States



MR-IMSRG: build correlations
already correlated state (e.g., fro
describes static correlation

use generalized normal ordering with 2B,... densities

MR-IMSRG References States

available

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- Generator Coordinate Method (with projections)
- small-scale No-Core Shell Model

future

- clustered states, Density Matrix Renormalization Group, tensor networks etc.

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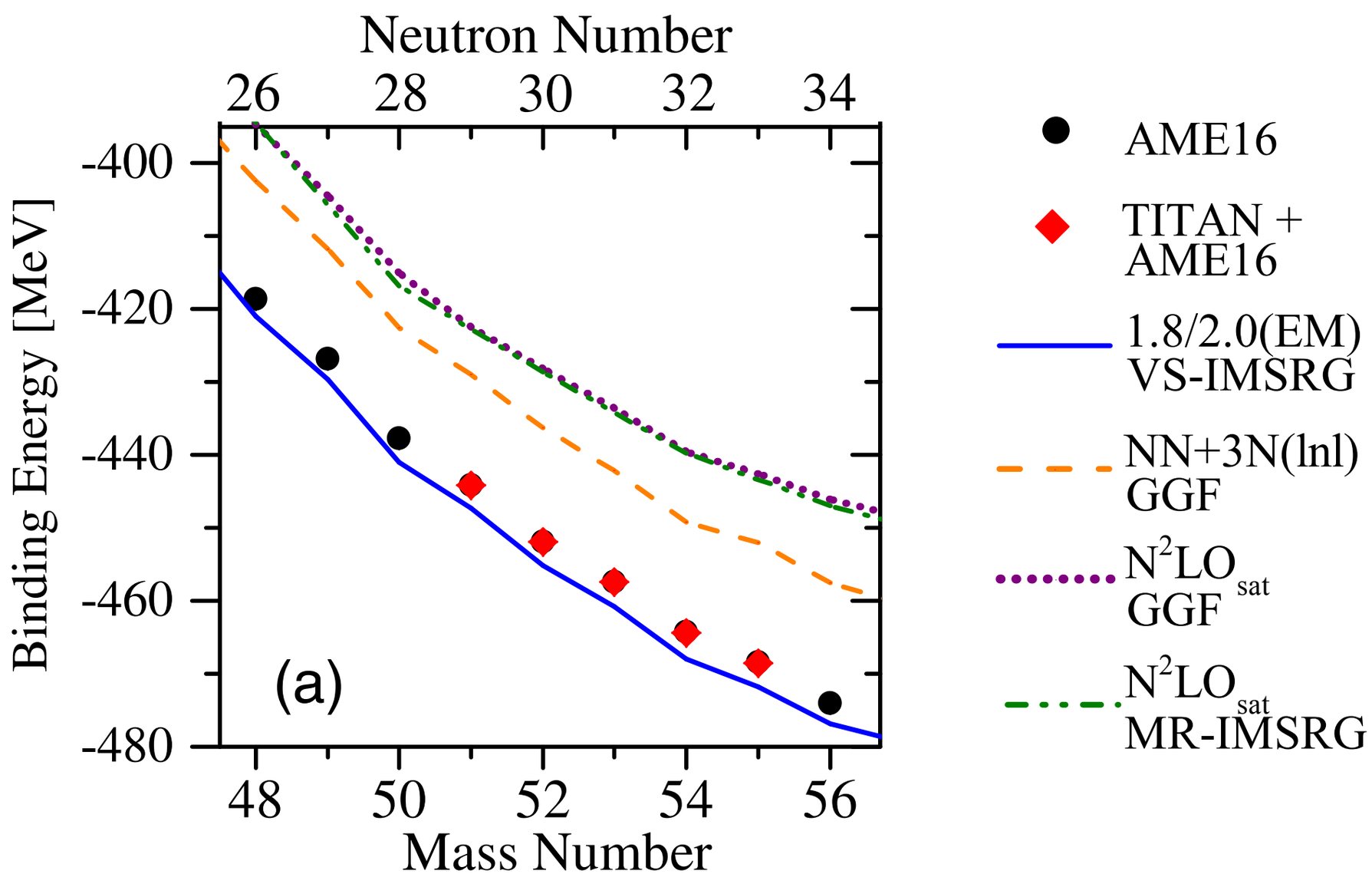
Titanium Isotopes

*E. Leistenschneider et al., PRL **120**, 062503 (2018)*



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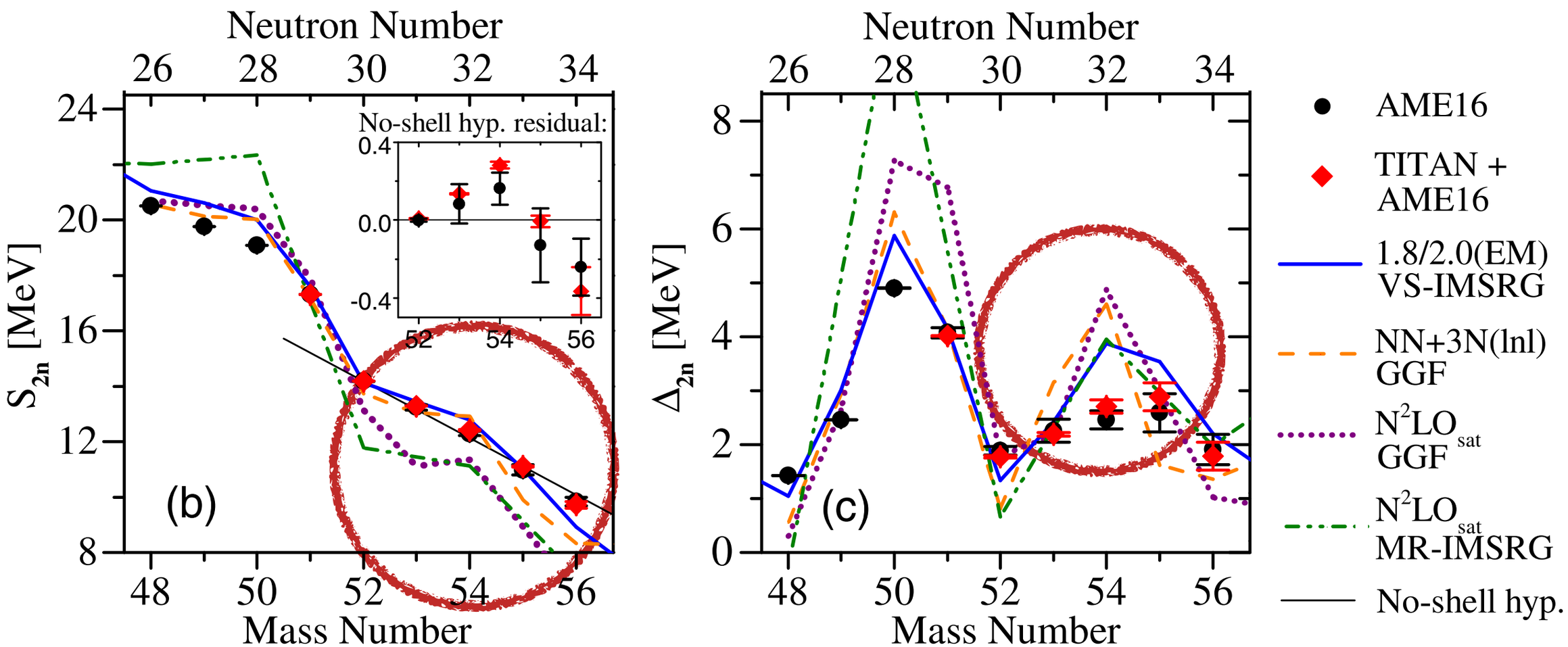
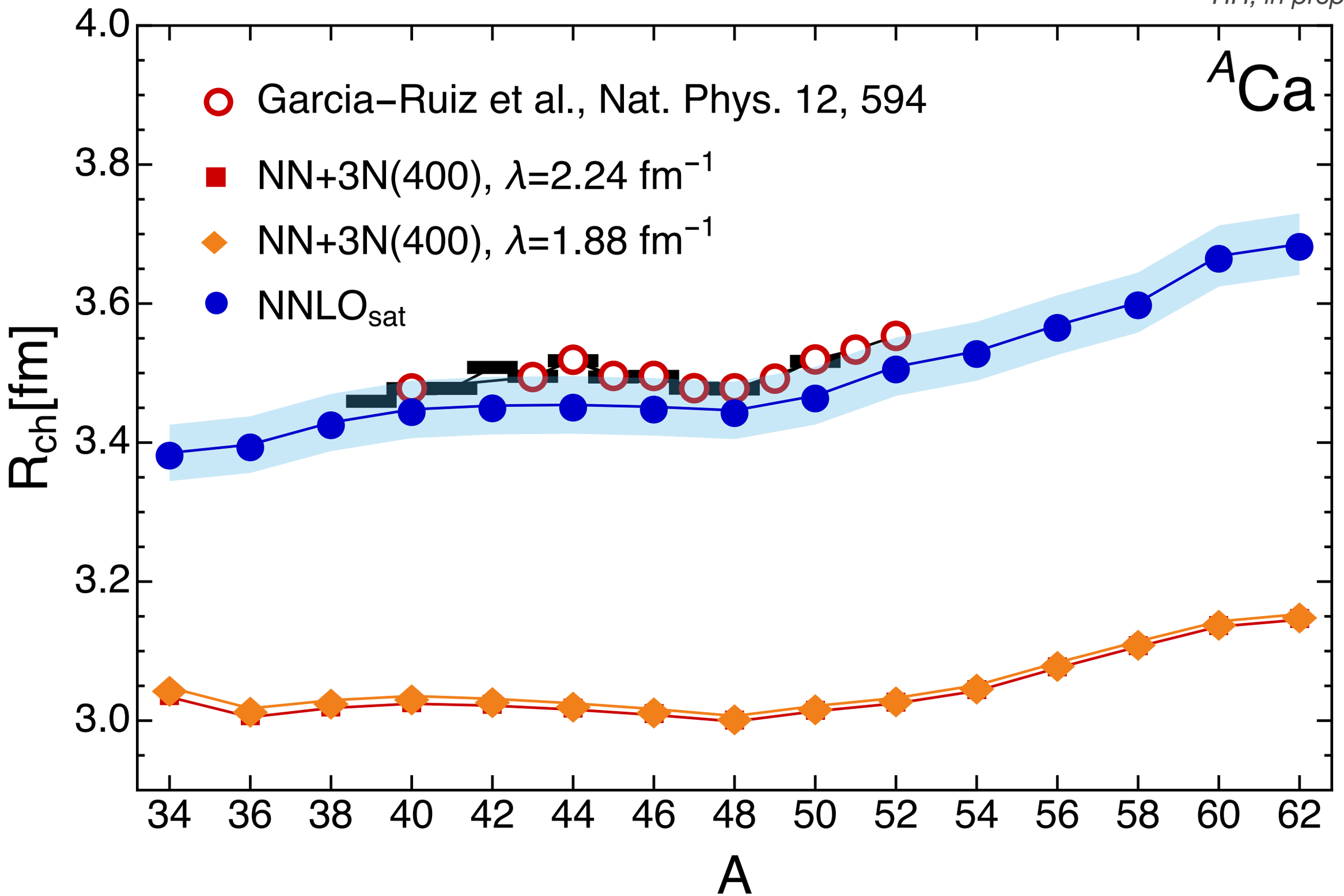


N=32 sub-shell **closure too pronounced**: combined effect of **method & interaction** !

Calcium Isotopes

HH, in preparation



Calcium Isotopes

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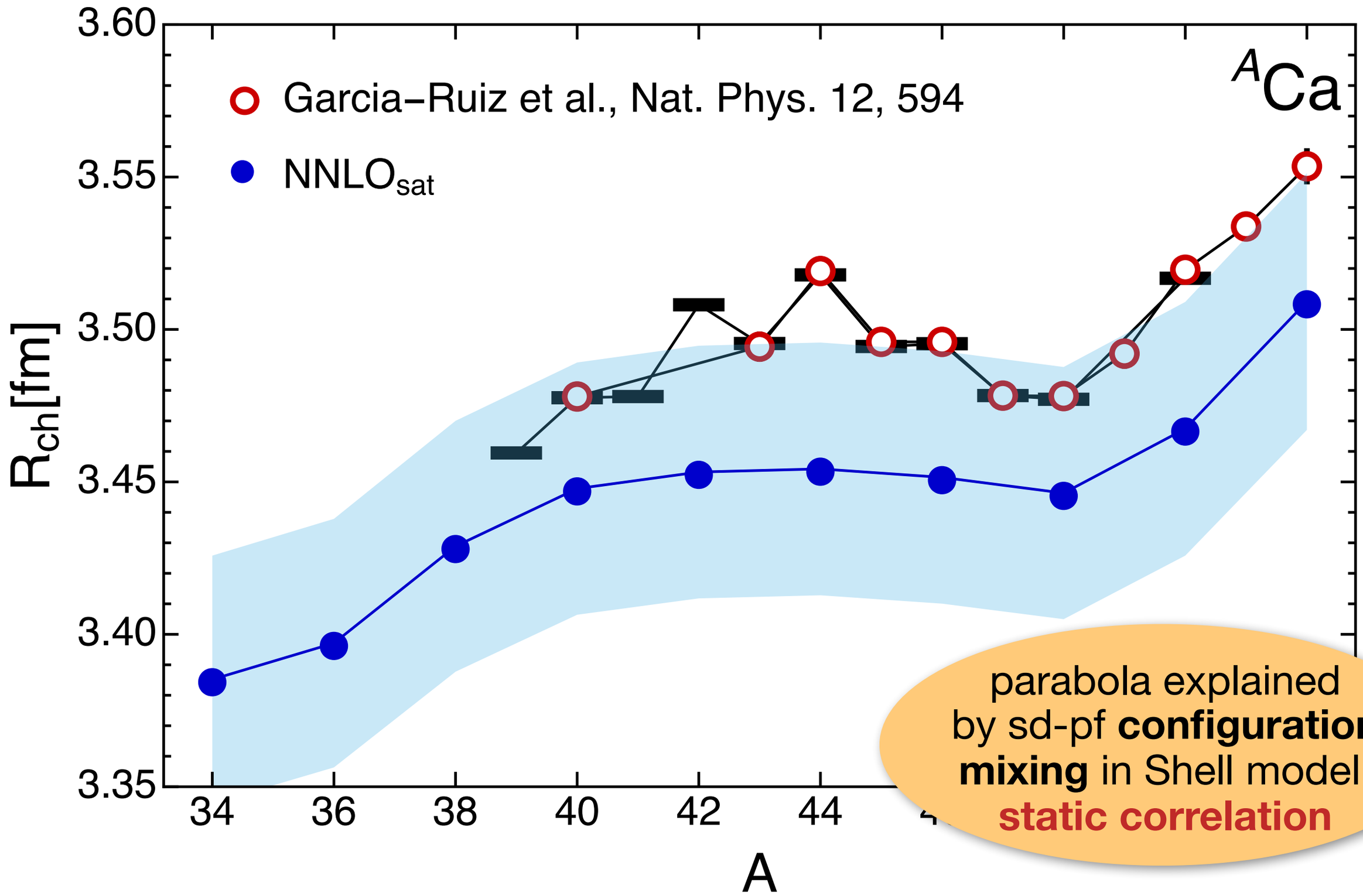

parabola explained by sd-pf **configuration mixing** in Shell model: **static correlation**

Excited States

N. M. Parzuchowski, T. D. Morris, S. K. Bogner, Phys. Rev. C **95**, 044304 (2017)

S. R. Stroberg, A. Calci, H. H., J. D. Holt, S. K. Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)

S. R. Stroberg, H. H., J. D. Holt, S. K. Bogner, A. Schwenk, Phys. Rev. C **93**, 051301(R) (2016)

S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. **113**, 142501 (2014)

MR-IMSRG References States

available

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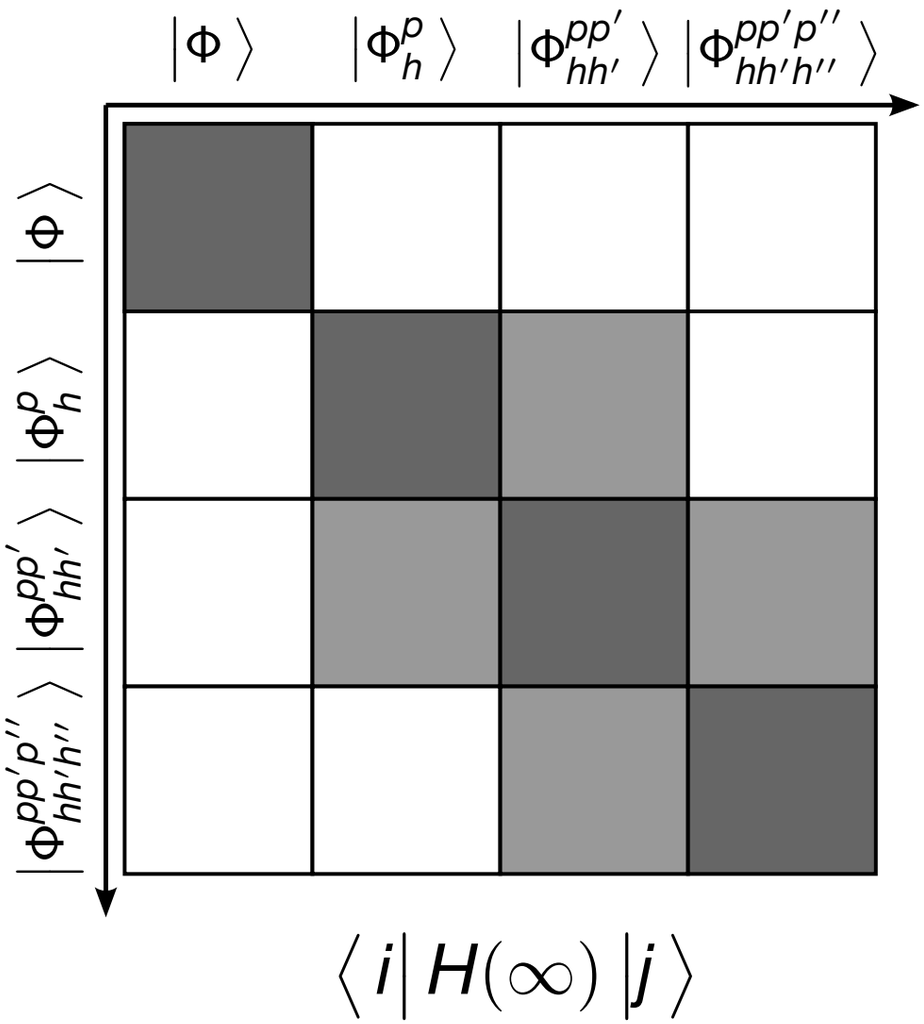
- Generator Coordinate Method (with projections)
- small-scale No-Core Shell Model

future

- clustered states, Density Matrix Renormalization Group, tensor networks etc.

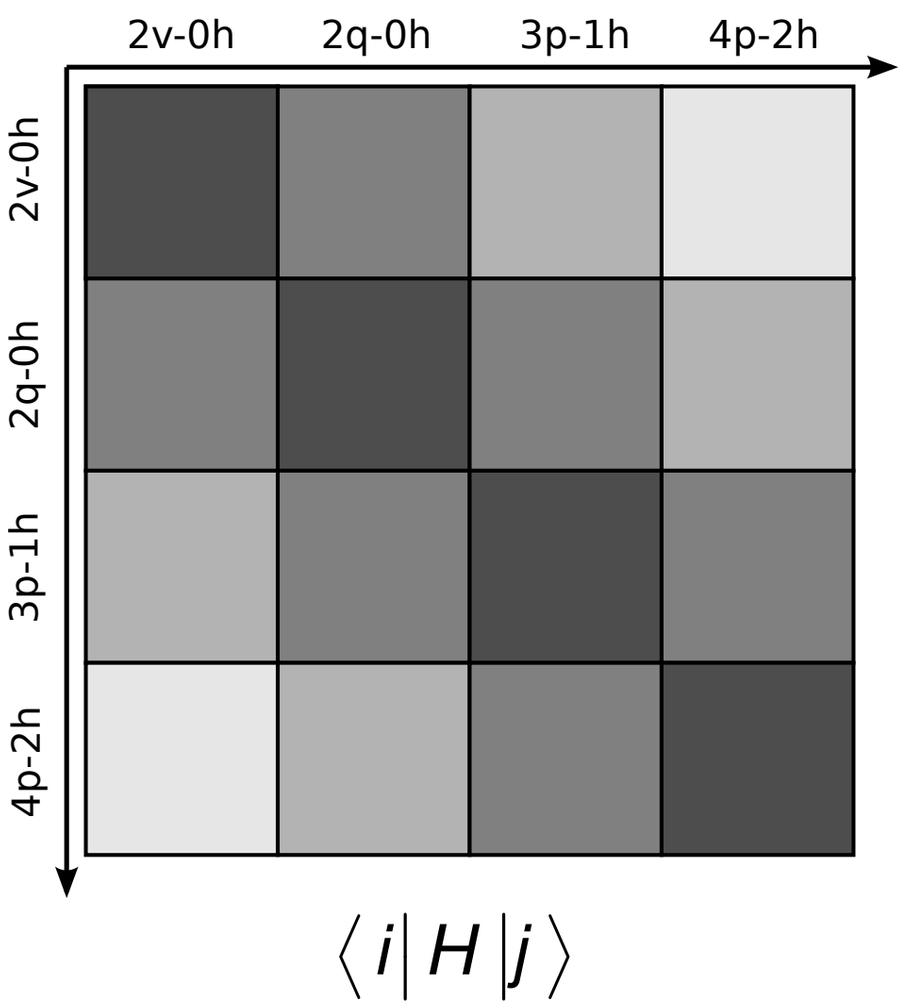
EOM-IMSRG

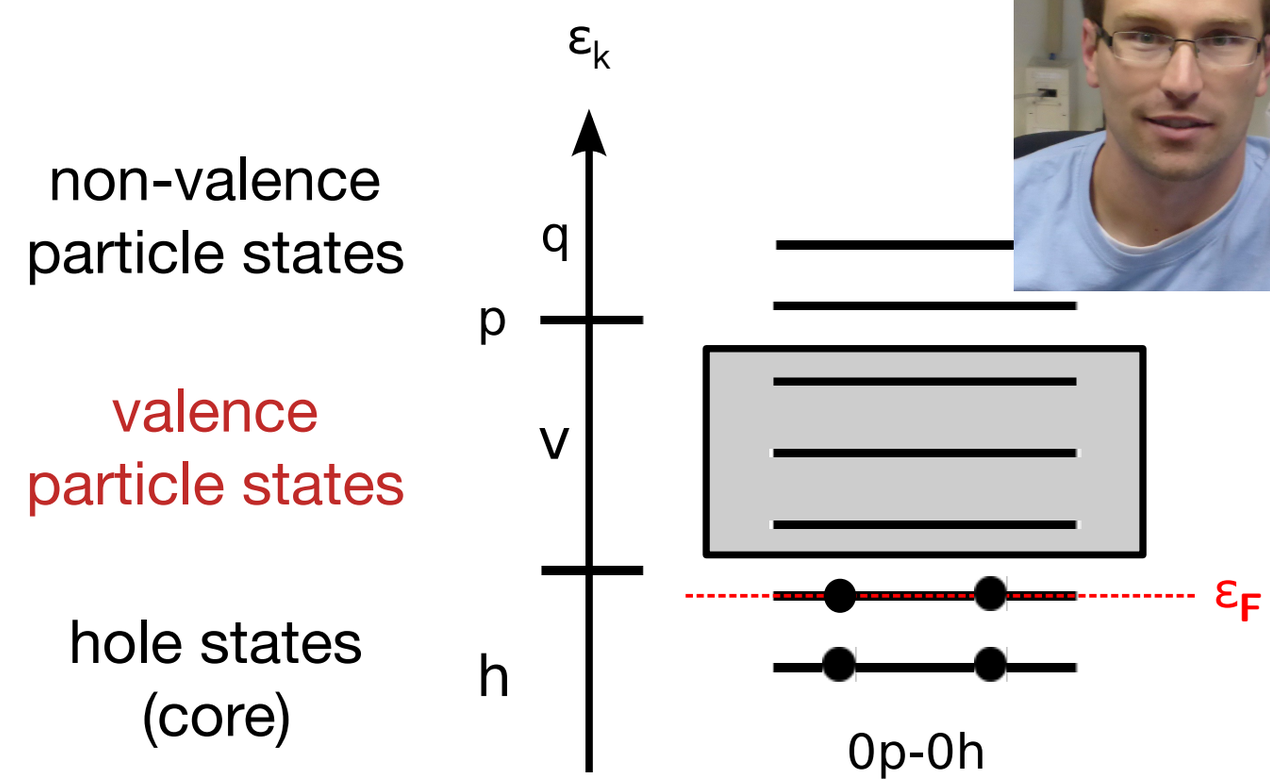
EOM-IMSRG: ***N. M. Parzuchowski*** *et al., PRC* ***95****, 044304*



- use IMSRG Hamiltonian as input for **Equation-of-Motion** approach
- **all nucleons active**
- currently include up to **2p2h excitation operators**

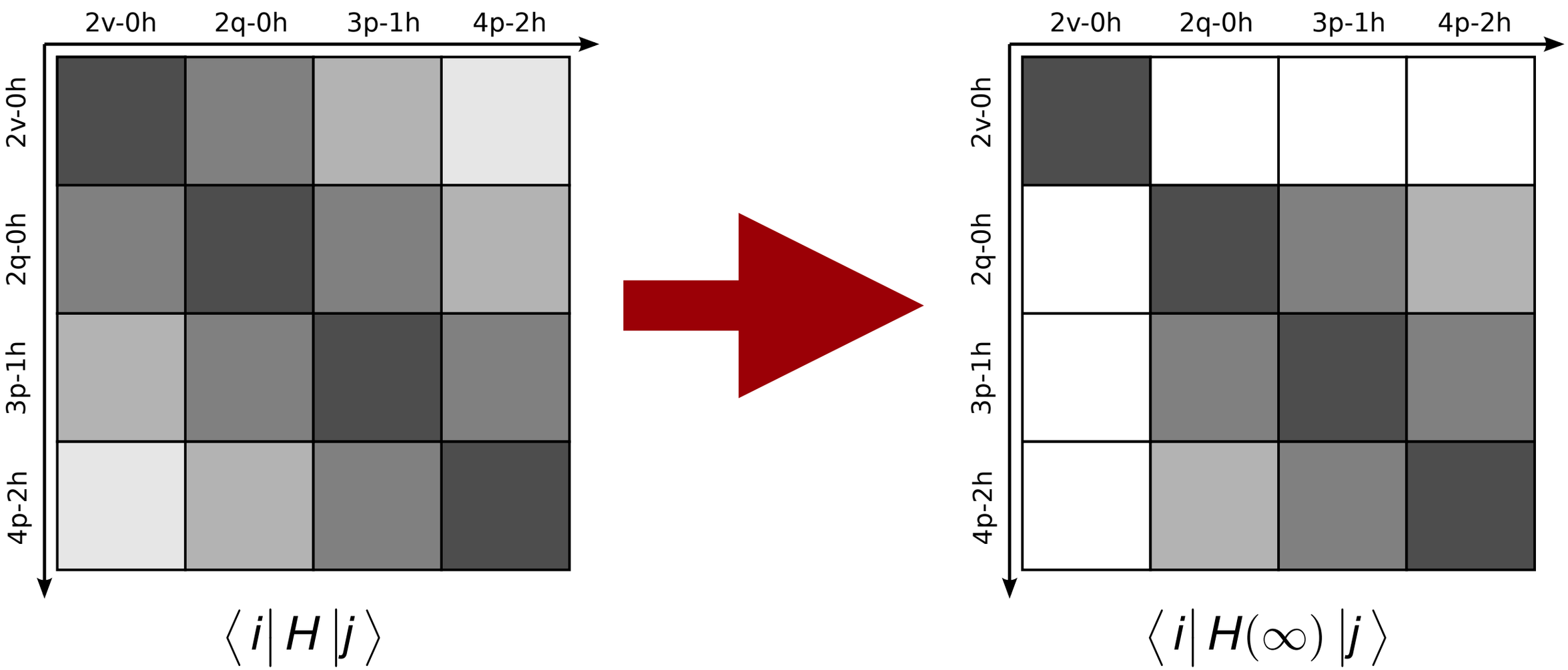
Valence Space Decoupling





construct **non-empirical interactions** (and other operators) for use in the nuclear **configuration interaction** method

Valence Space Decoupling

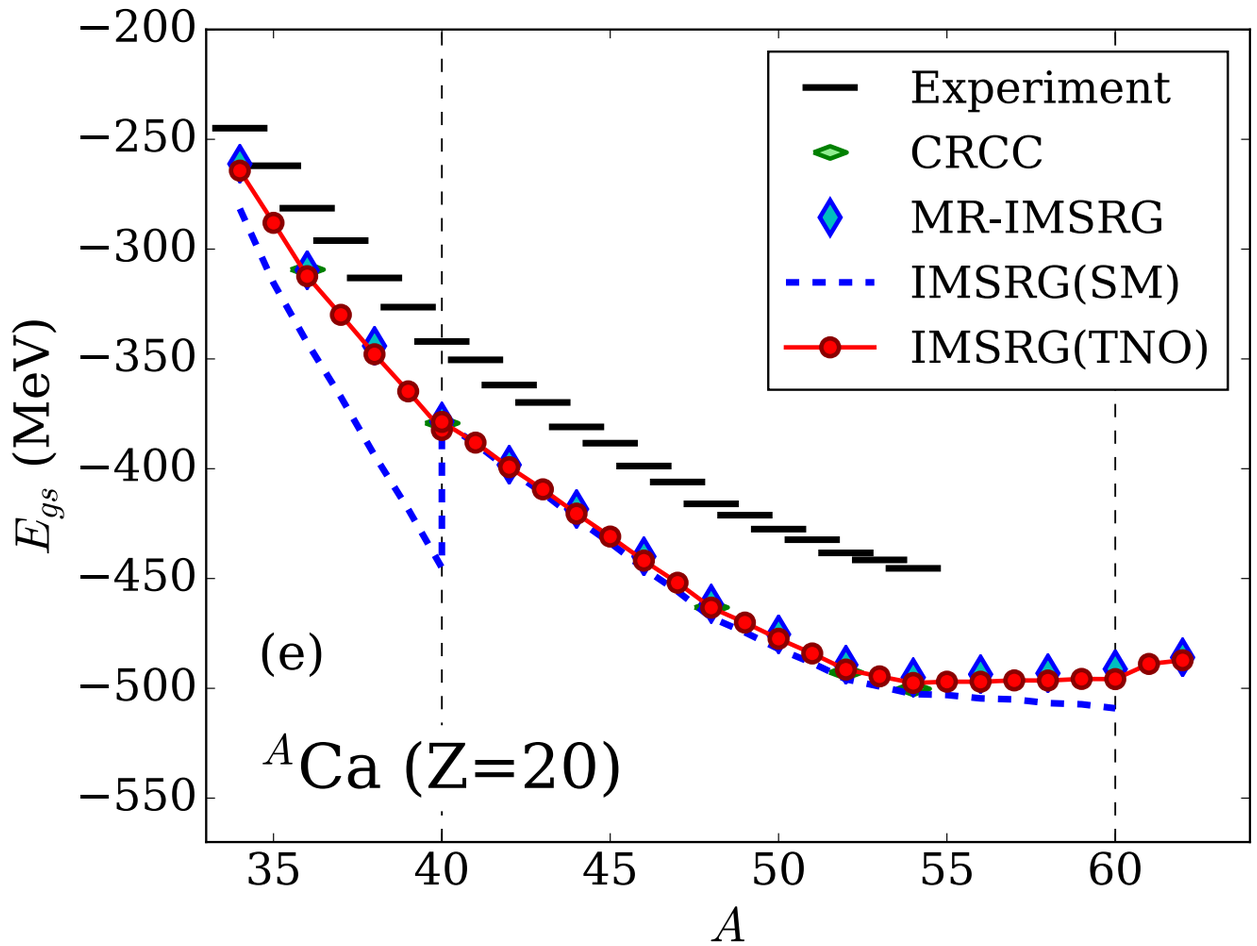


change definition of off-diagonal Hamiltonian:

$$\left\{H^{od}\right\} = \{f^{h}_{h'}, f^{p}_{p'}, f^{p}_{h}, f^{q}_{v}, \Gamma^{pp'}_{hh'}, \Gamma^{pp'}_{hv}, \Gamma^{pq}_{vv'}\} \text{ \& H.c.}$$

Ground-State Energies

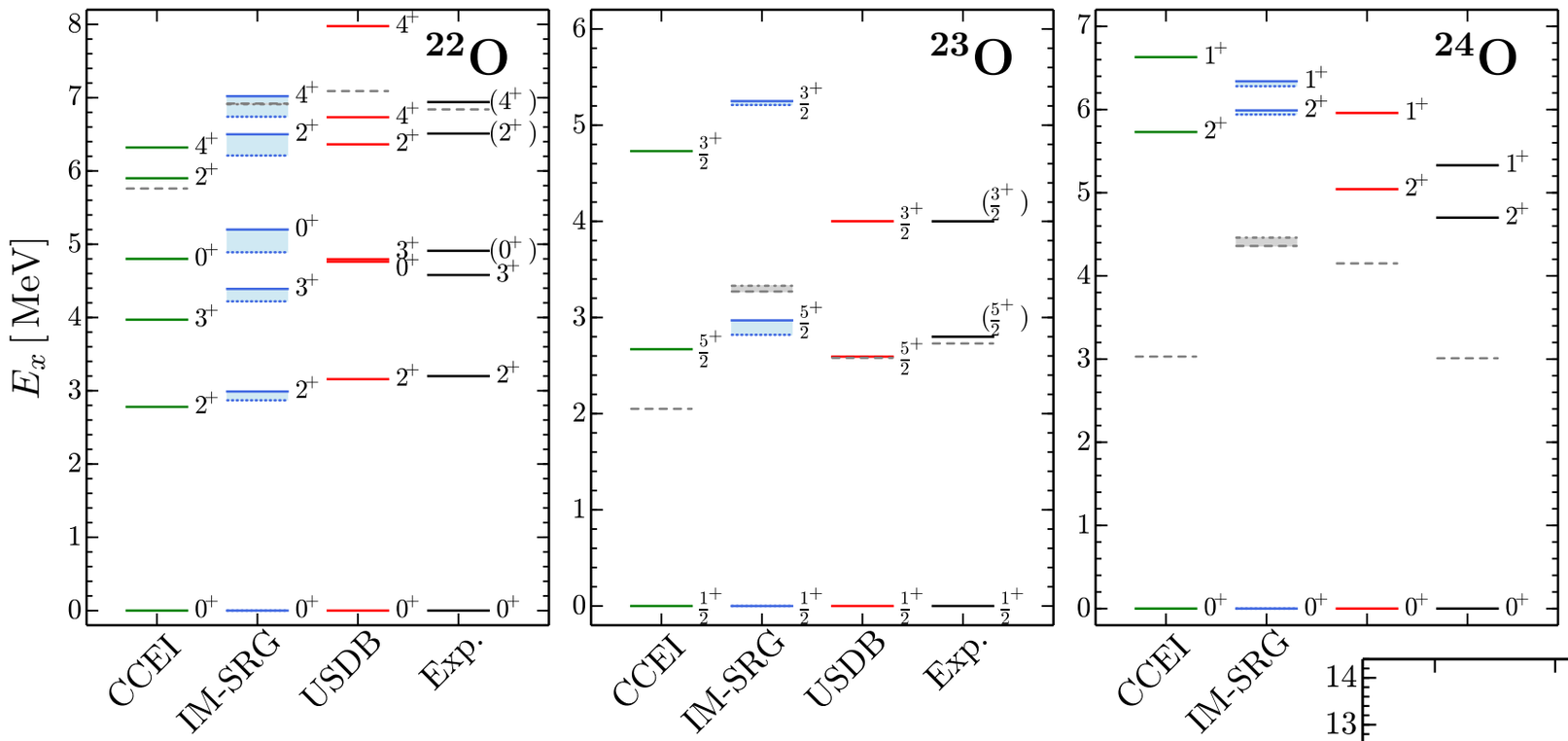
*S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)*

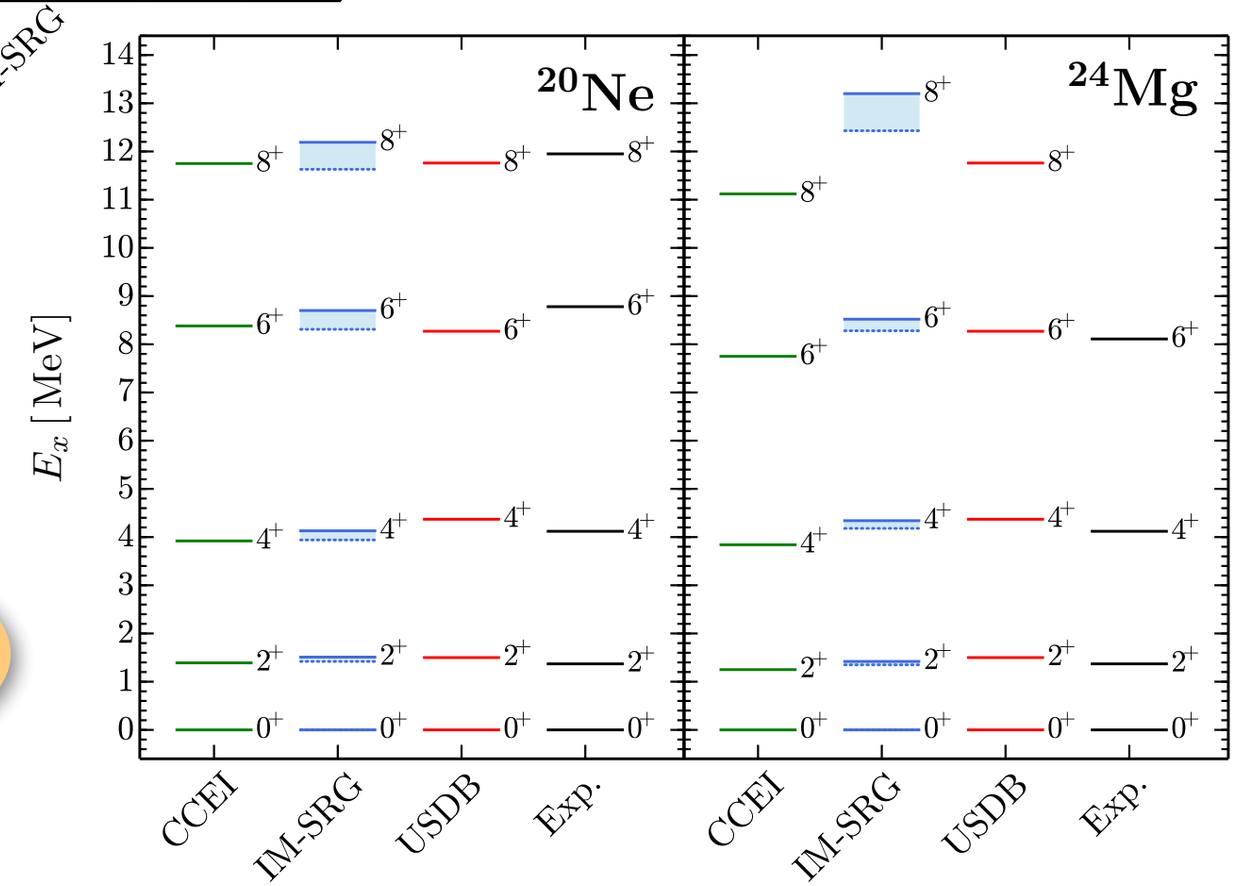


- (initial) normal ordering and IMSRG decoupling in the **target nucleus**
- **consistent with (MR-)IMSRG ground state energies** (and CC, SCGF, …) for the **same Hamiltonian**

Excitation Spectra

*S. K. Bogner et al., PRL **113**, 142501 (2014), S. R. Stroberg et al., PRC **93**, 051301(R) (2016)*



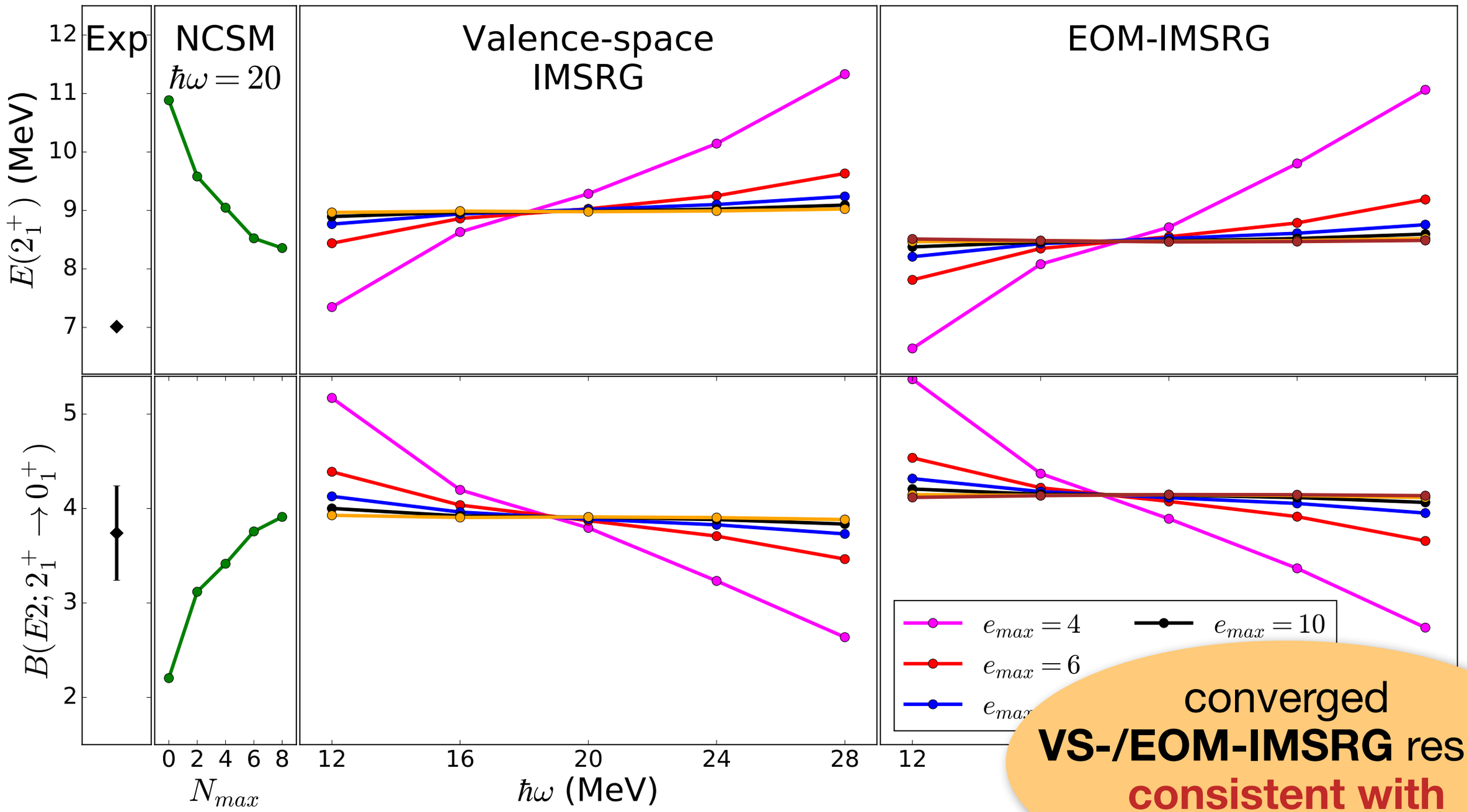


sd-shell spectra agree very well with experiment and USDA/B…

… for NN+3N(400) with "wrong" c_D = -0.2.

Transitions

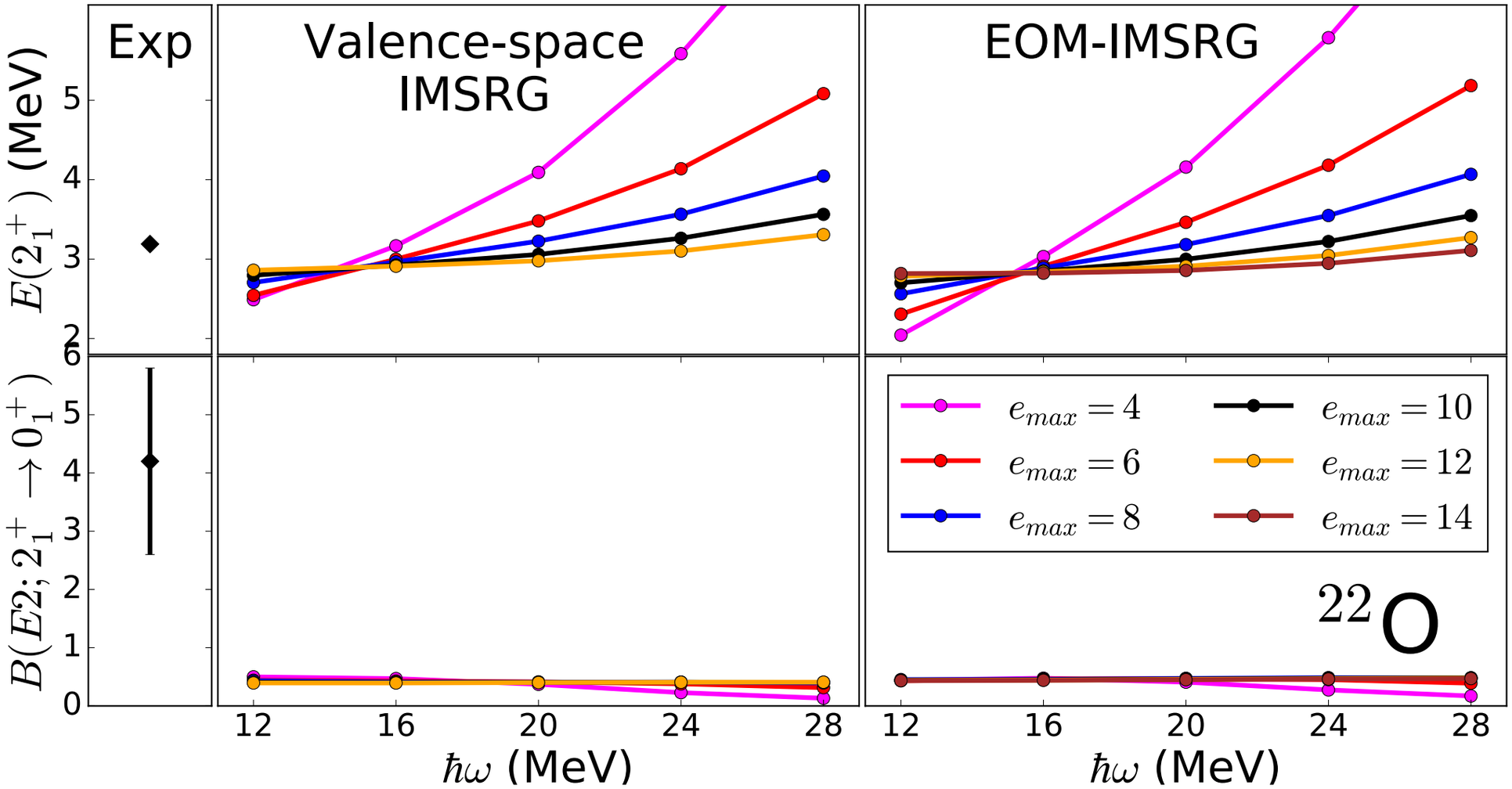
N. M. Parzuchowski, *S. R. Stroberg et al., PRC* ***96****, 034324;*



converged **VS-/EOM-IMSRG** results **consistent with NCSM**

Transitions

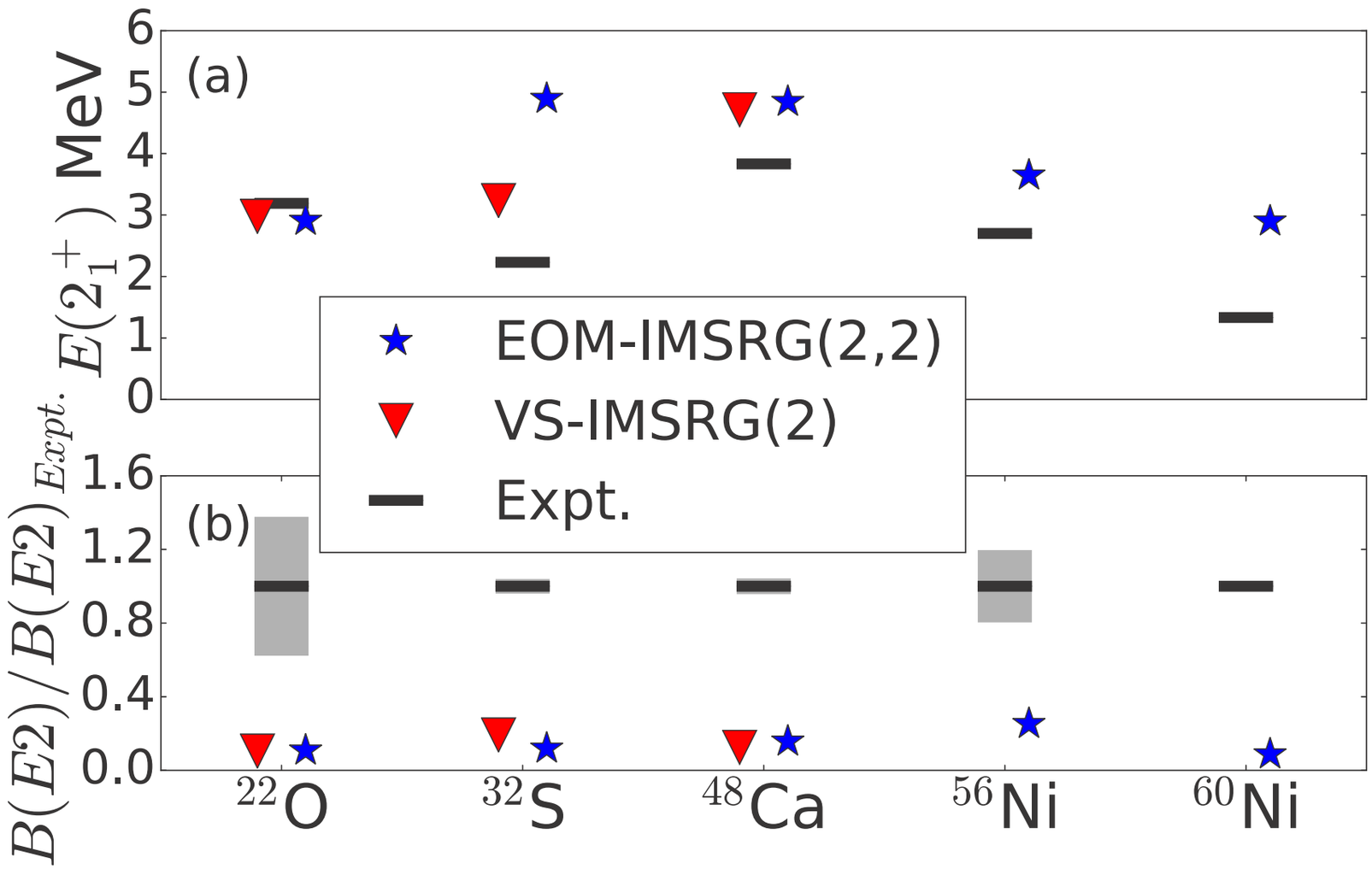
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324; EOM-IMSRG: N. M. Parzuchowski et al., PRC **95**, 044304*



- non-zero B(E2) from Shell model: **VS-IMSRG induces effective neutron charge**
- **B(E2) much too small:** effect of intermediate 3p3h, … states that are truncated in IMSRG evolution

Transitions

*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324*



- **B(E2) much too small:** effect of intermediate 3p3h, … states that are truncated in IMSRG evolution

Capturing Static Correlations: IMSRG+GCM

J. M. Yao, C. F. Jiao, L. J. Wang, J. Engel, H. H., *in preparation*

MR-IMSRG References States

available

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- **Generator Coordinate Method (with projections)**

future

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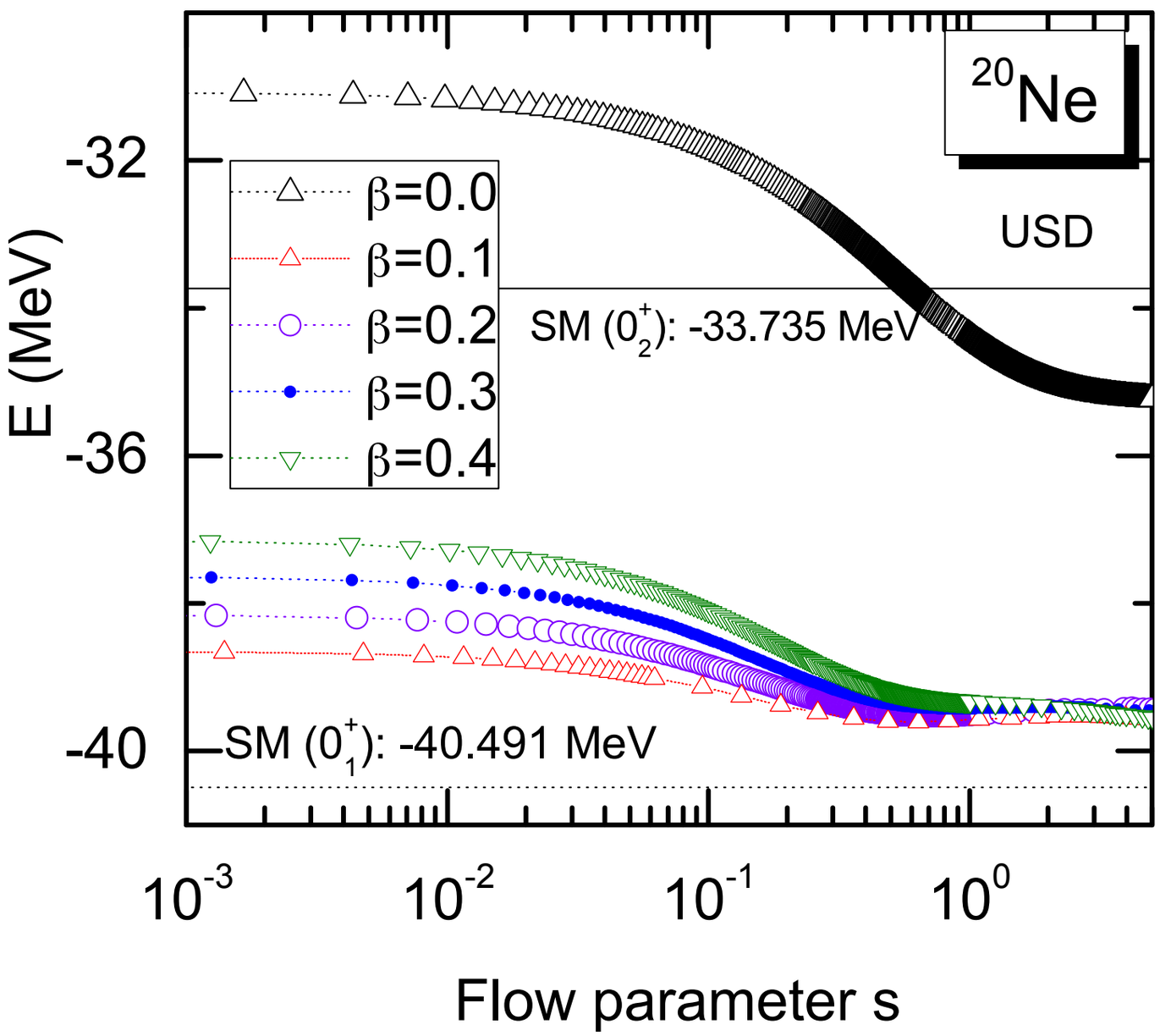
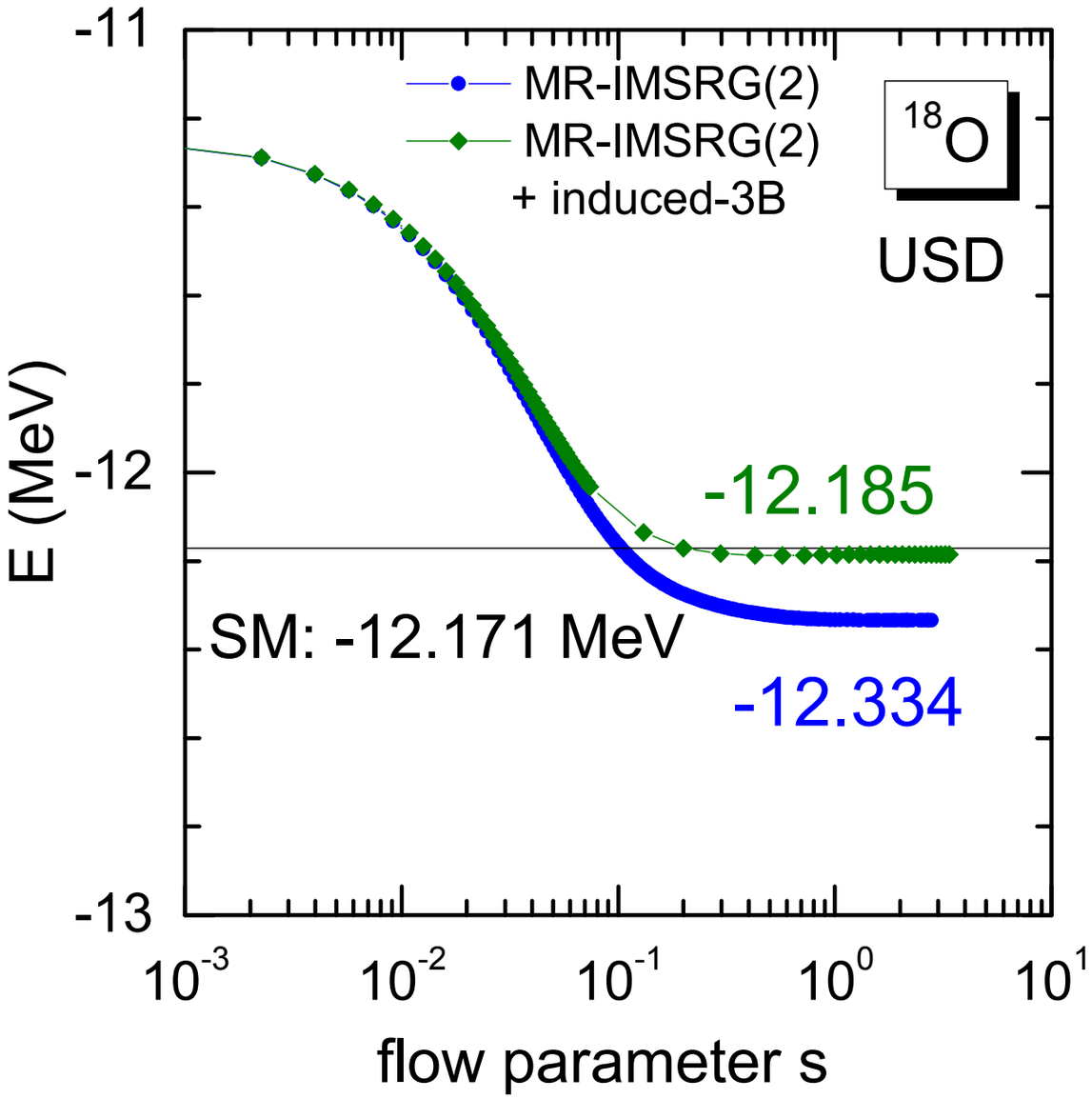
- clustered states, Density Matrix Renormalization Group, tensor networks etc.

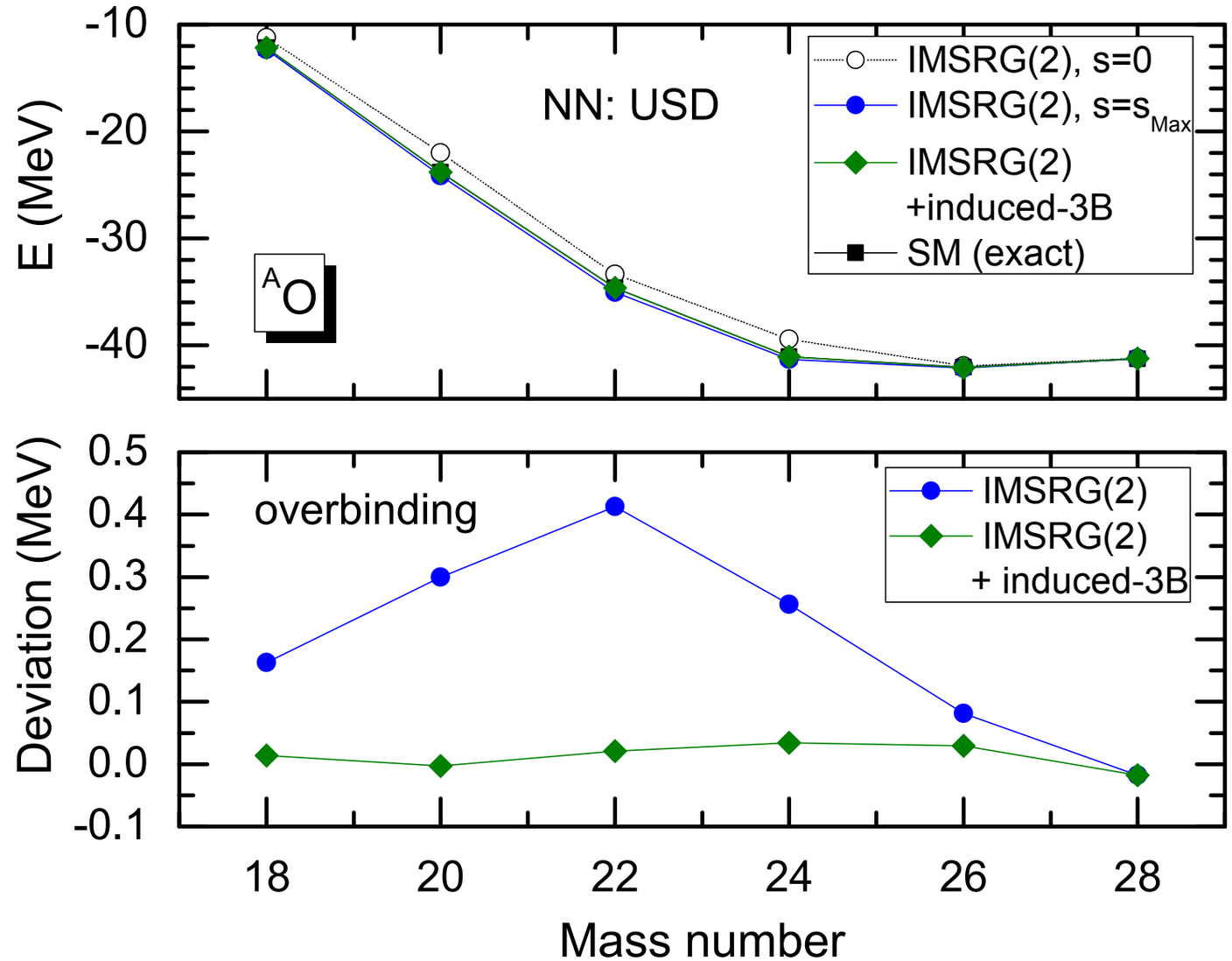
Example: ^{20}Ne



- reference: particle-number & angular-momentum projected HFB
- **range of deformed reference states flow to the ^{20}Ne ground state**
- deviation from Shell model result: **correlations beyond MR-IMSRG(2)**

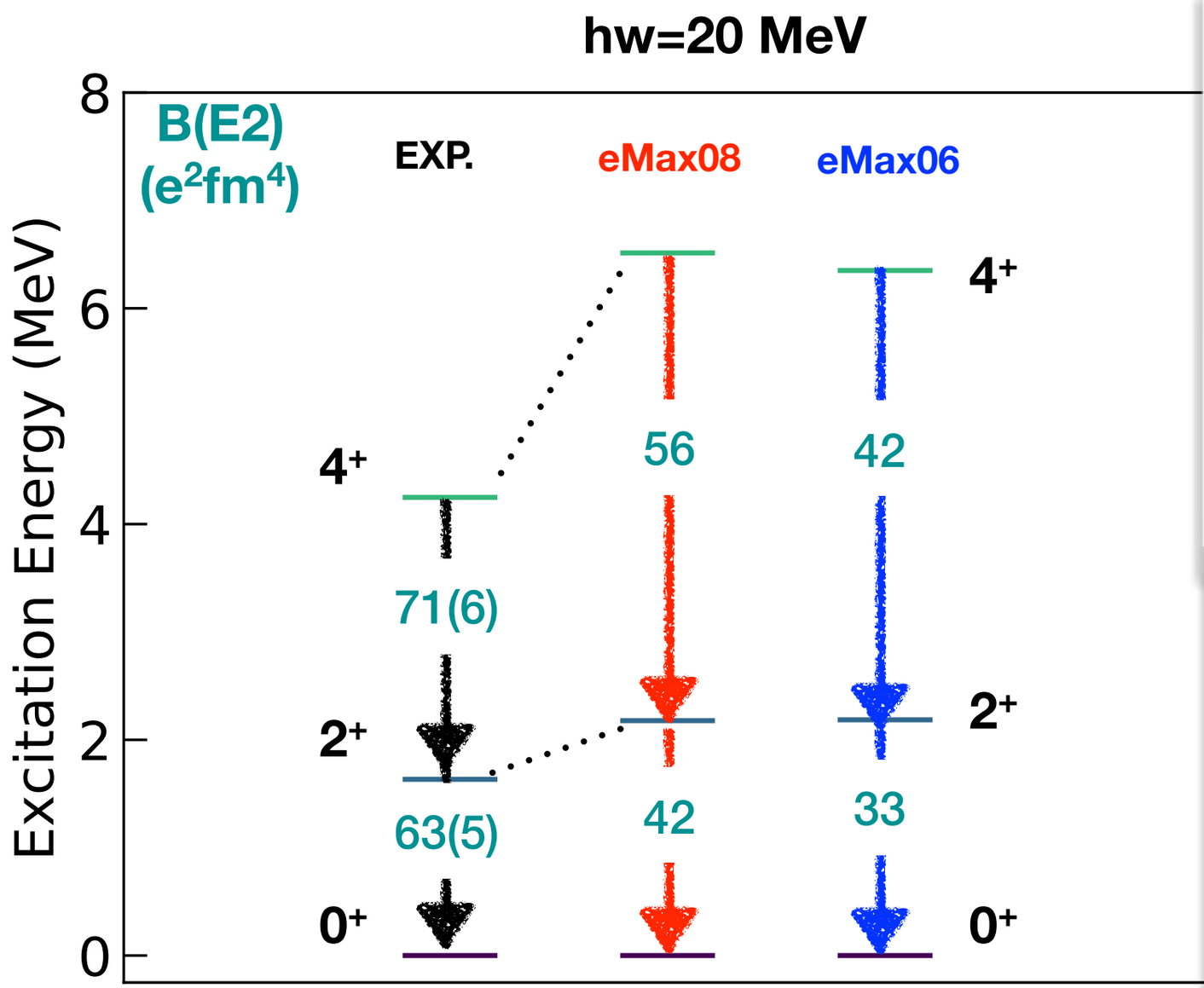
Approximate MR-IMSRG(3)

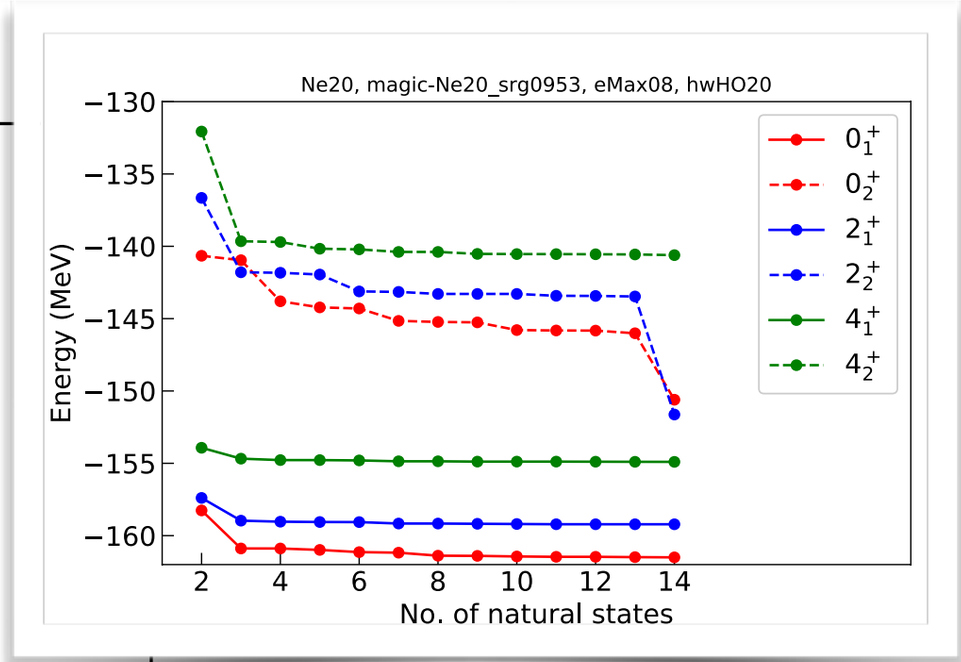


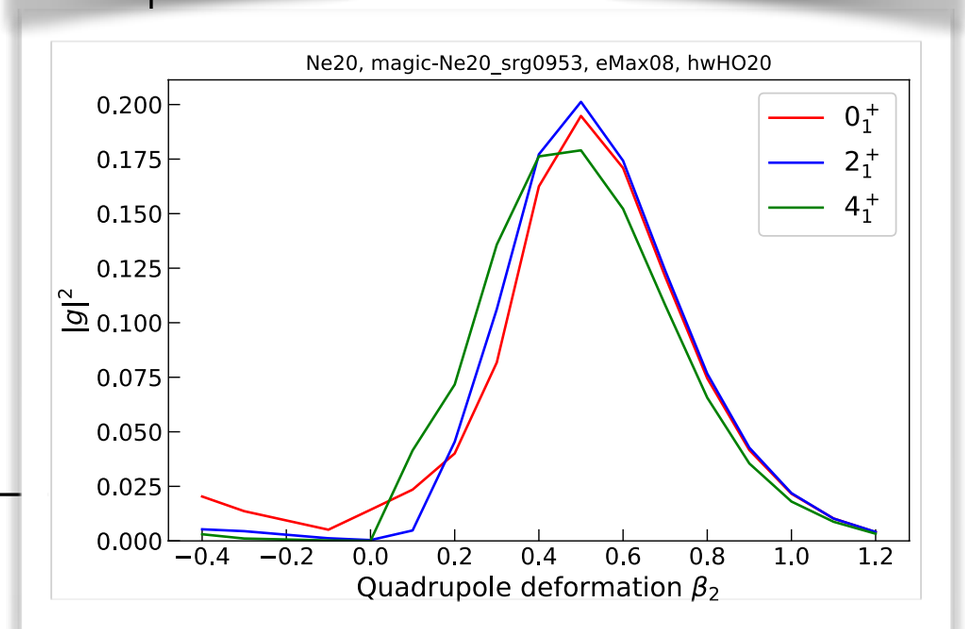


- **approximate MR-IMSRG(3):** induced 3B terms recover bulk of missing correlation energy
- size will be **reference-state dependent**

IMSRG+GCM for ^{20}Ne







- rotational band spread out
- B(E2) **significantly boosted,** but still underestimated (2B part of effective E2 not included yet, spectrum spread out)

Merging IMSRG and NCSM

E. Gebrerufael, **K. Vobig**, HH and R. Roth, *in preparation*

E. Gebrerufael, **K. Vobig**, HH and R. Roth, PRL **118**, 152503 (2017)

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future

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Concept

*E. Gebrerufael, K. Vobig, HH and R. Roth, PRL **118**, 152503 (2017)*

NCSM
define
reference state

- diagonalization in small model space
- use eigenstate as reference

IMSRG
evolve
operators

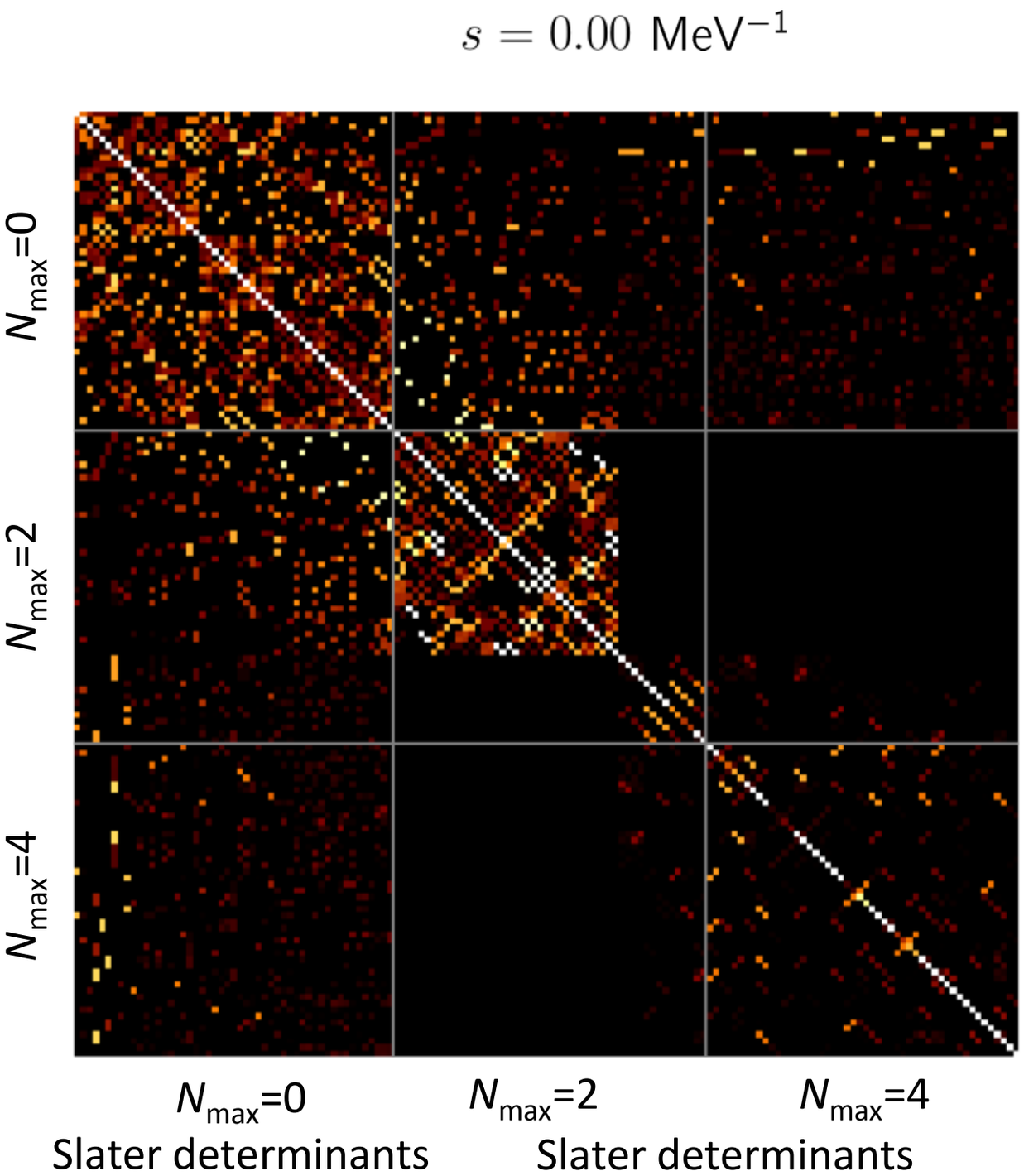
- evolve Hamiltonian and observables with MR-IMSRG
- decoupling in A-body space

NCSM
extract
observables

- diagonalize evolved Hamiltonian
- calculate eigenstates, observables

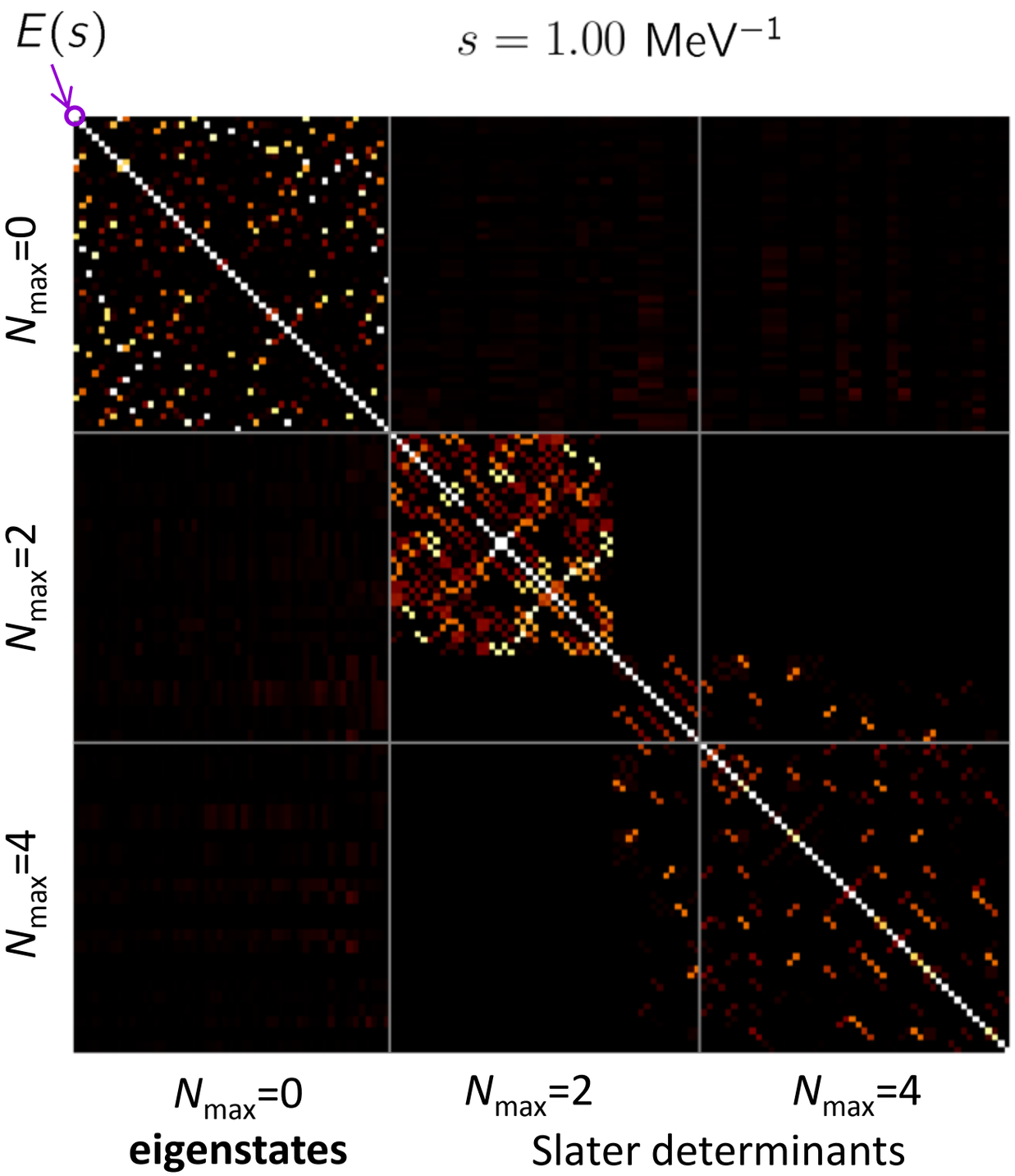
^{12}C: Hamiltonian Matrix Evolution

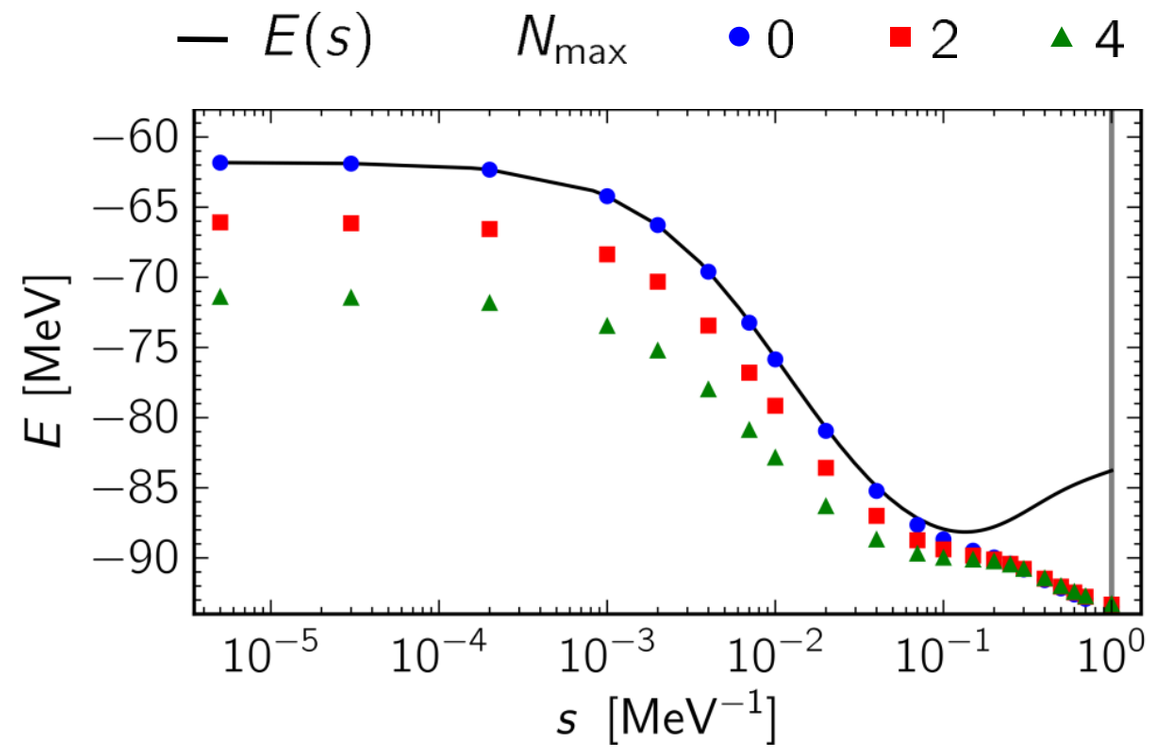
figures by E. Gebrerufael



^{12}C: Hamiltonian Matrix Evolution

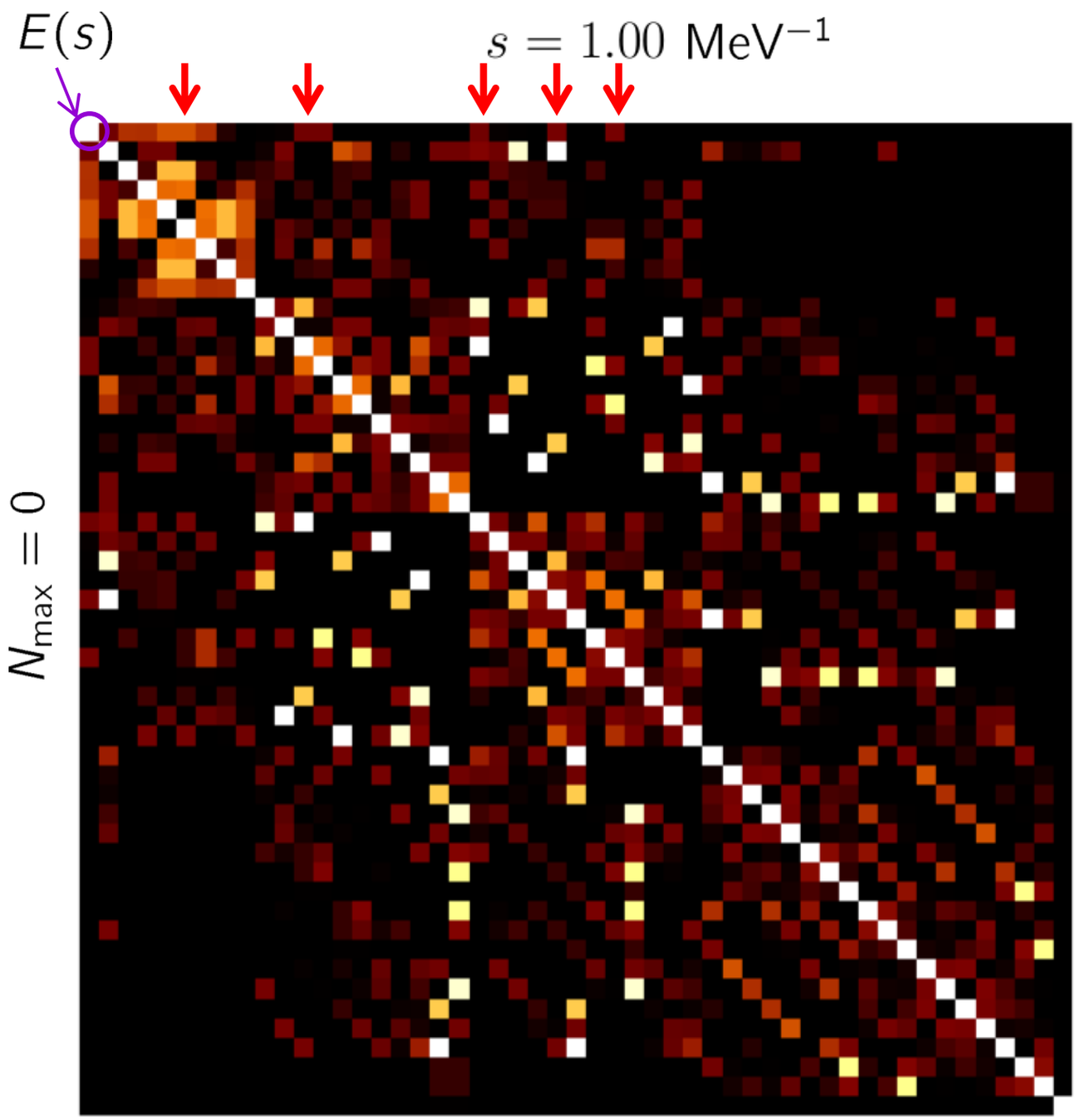
figures by E. Gebrerufael





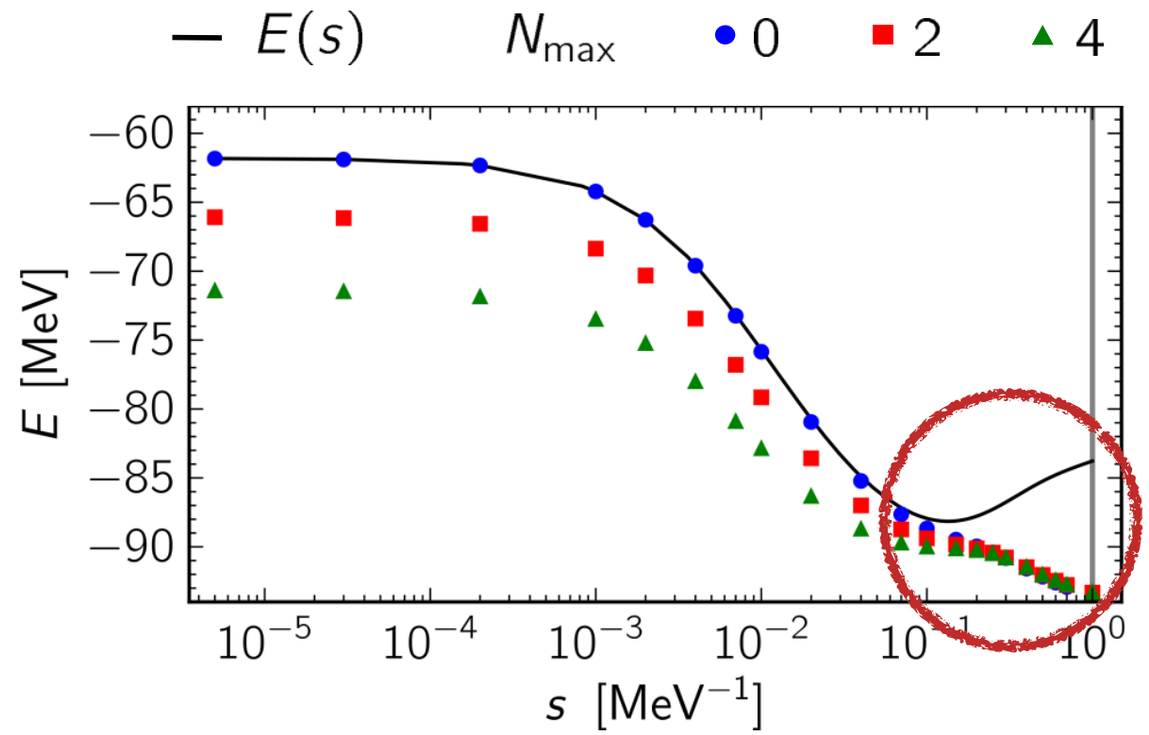
- N_{max}=0,2,4 eigenvalues (almost) **identical due to decoupling**…
- … but **IMSRG truncation artifacts** appear eventually (missing induced 3B+ terms)

Evolution of the Hamiltonian Matrix



N_{max}=0
eigenstates

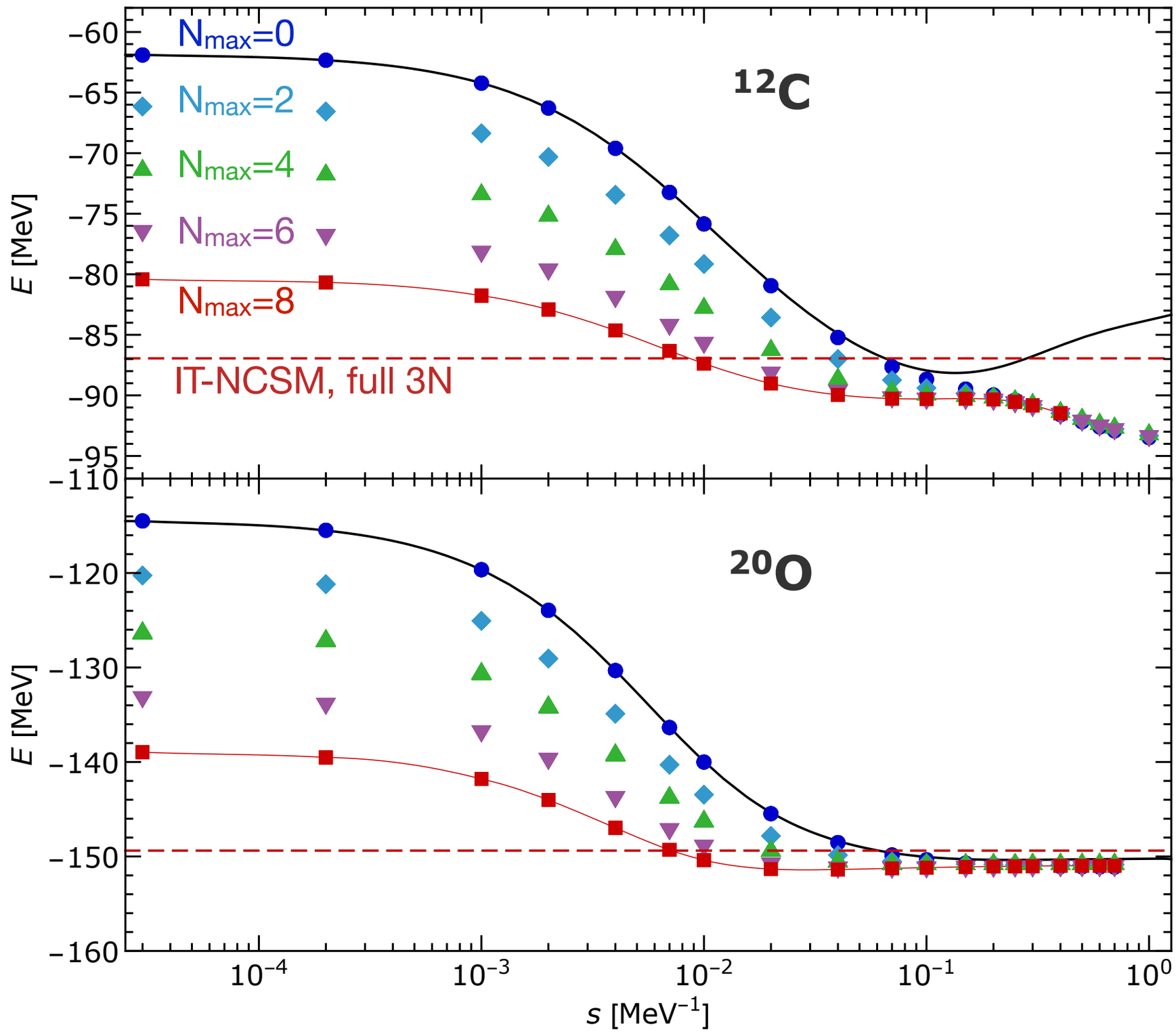
figures by E. Gebrerufael



- **induced couplings** between reference and N_{max}=0 states
- E(s) does not track lowest eigenvalue

➡ **diagonalize H(s)**

Evolution of Ground-State Energies

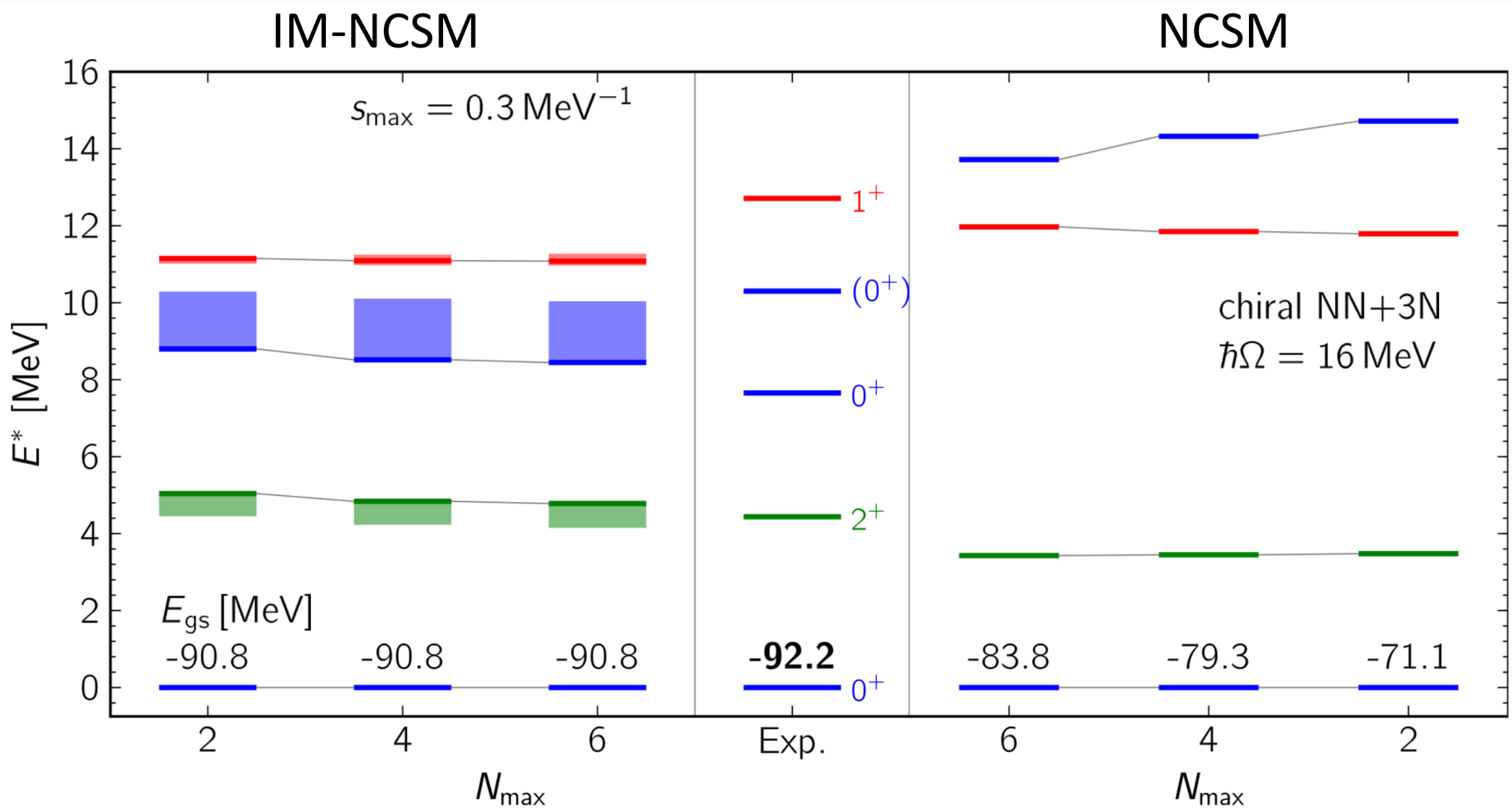


EM 500/400
NO2B
$\lambda = 1.88$ fm^{-1}
$\hbar\Omega = 20$ MeV

N_{max} = 0,2,4,6,8

- **strongly enhanced convergence**
- **plateau** in flow
- identify **critical s_{max}** at which **induced many-body** terms become **relevant**

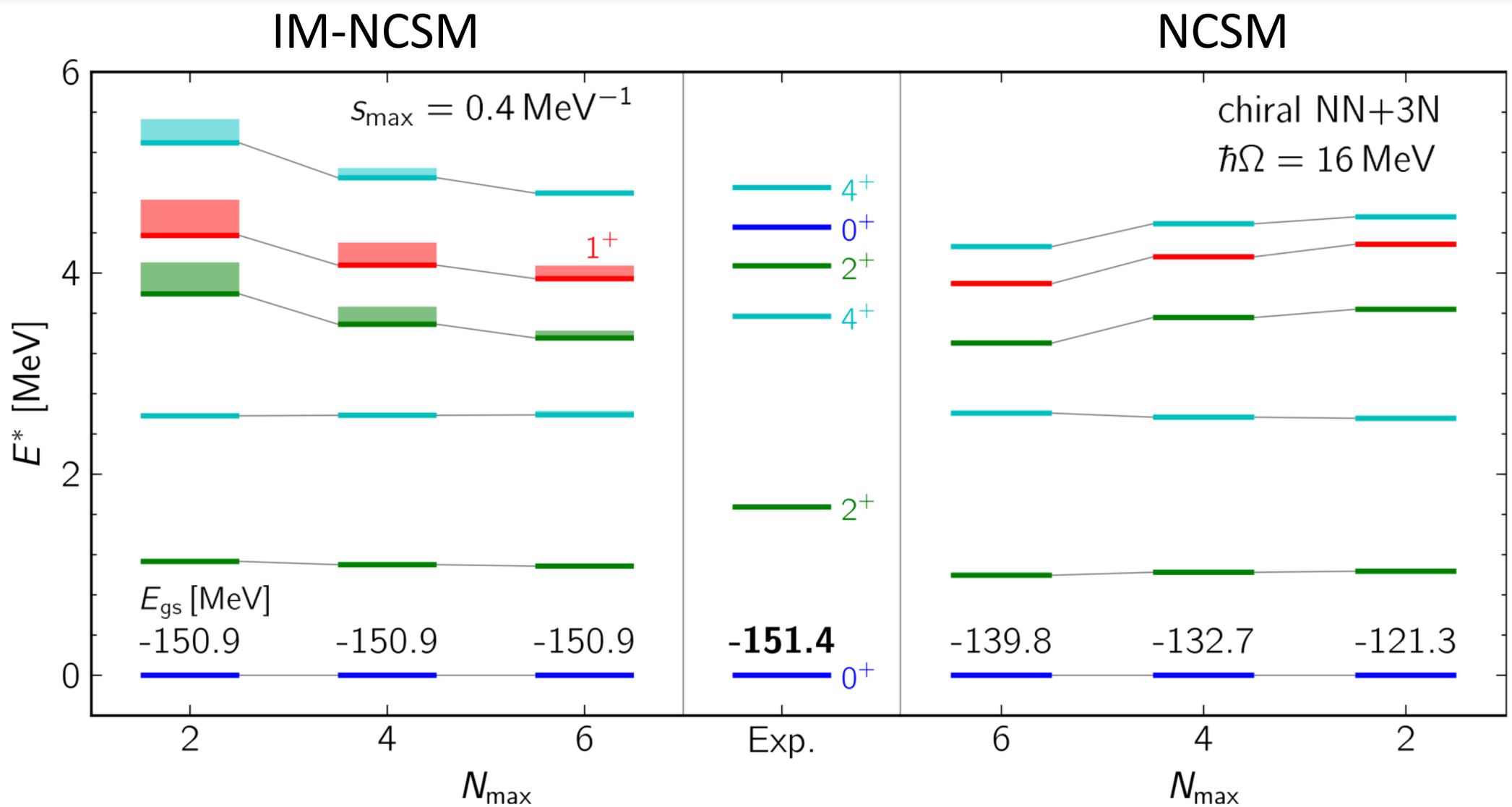
^{12}C: Excitation Spectra



EM 500/400
NO2B
$\lambda = 1.88\ \mathrm{fm}^{-1}$
$\hbar\Omega = 20$ MeV

- "uncertainty band": **flow parameter variation** from $s_{max}/2$ to s_{max}
- **excellent agreement for converged states**

^{20}O: Excitation Spectra



EM 500/400
NO2B
$\lambda = 1.88\ \mathrm{fm}^{-1}$
$\hbar\Omega = 20$ MeV

- excellent agreement for converged states
- **predict 1^+ state** that has not yet been observed experimentally

Epilogue

Where Do We Go from Here?

- Revisit **optical potentials** (à la J. Rotureau et al., PRC 95, 024315)
  - MR-EOM / GCM / … to describe **few-particle and collective** correlation
  - **continuum coupling** for exotic nuclei (see K. Fossez)
- Use **IMSRG-evolved Hamiltonians** in RGM/NCSMC/…)
- **Utopia:** Can we **systematically** connect many-body system to few-body system via IMSRG (or other RG) methods?

Acknowledgments

S. K. Bogner, K. Fossez, J. Hill, M. Hjorth-Jensen, **J. M. Yao**
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UT Knoxville & Oak Ridge National Laboratory

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